



STIC Search Report

EIC 1700

STIC Database Tracking Number: 190809

TO: Dawn Garrett
Location: REM 10C79
Art Unit : 1774
May 25, 2006

Case Serial Number: 10/518713

From: Usha Shrestha
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-3519
usha.shrestha@uspto.gov

Search Notes

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: DAWN GARRETT Examiner #: 76107 Date: 5/22/2006
 Art Unit: 1774 Phone Number 302-1523 Serial Number: 10/518,713
 Mail Box and Bldg/Room Location: Remain 10C79 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Polymer and polymeric luminescent element
 Inventors (please provide full names): Comprising the same

(see attached Bil. data sheet)

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search a polymer according to
 claim 1
 (do not limit by utility)

Thank you.

SCIENTIFIC REFERENCE BR
 Sci & Tech Inf. Cntr.

MAY 23 2006

Pat. & T.M. Office

STAFF USE ONLY

Type of Search		Vendors and cost where applicable
Searcher: <u>WJL</u>	NA Sequence (#) _____	STN <u>670.99</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>1</u>	Questel/Orbit _____
Date Searcher Picked Up: <u>5/25/06</u>	Bibliographic _____	Dr.Link _____
Date Completed: <u>5/25/06</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>30</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: <u>30</u>	Patent Family _____	WWW/Internet _____
Online Time: <u>60</u>	Other _____	Other (specify) _____

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FILE 'REGISTRY' ENTERED AT 15:02:28 ON 25 MAY 2006

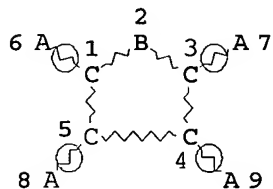
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L2 SCR 1847
L3 237 SEA FILE=REGISTRY SSS FUL L1 NOT L2
L4 3 S L3 AND PMS/CI

FILE 'HCAPLUS' ENTERED AT 15:04:12 ON 25 MAY 2006

L5 3 S L4
L6 103 S L3
L7 100 S L6 NOT L5
L8 19 S L7 AND P/DT
L9 11 S L8 AND (1907-2002)/PRY,AY
L10 81 S L7 NOT L8
L11 66 S L10 NOT (2003-2006)/PY
L12 77 S L9 OR L11

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L1 STR



NODE ATTRIBUTES:

NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L2 SCR 1847
L3 237 SEA FILE=REGISTRY SSS FUL L1 NOT L2
L4 3 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND PMS/CI
L5 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L4

=> fil hcap

FILE 'HCAPLUS' ENTERED AT 15:06:36 ON 25 MAY 2006

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L5 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:125112 HCAPLUS

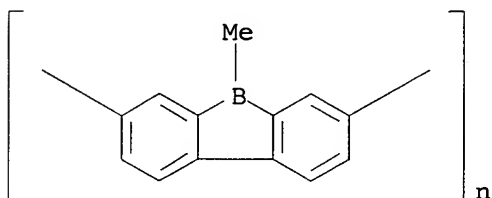
DOCUMENT NUMBER: 140:322032
 TITLE: Electronic, Structural, and Optical Properties of Conjugated Polymers Based on Carbazole, Fluorene, and Borafluorene
 AUTHOR(S): Briere, Jean-Francois; Cote, Michel
 CORPORATE SOURCE: Departement de Physique et Regroupement Quebecois sur les Materiaux de Pointe (RQMP), Universite de Montreal, Montreal, QC, H3C 3J7, Can.
 SOURCE: Journal of Physical Chemistry B (2004), 108(10), 3123-3129
 CODEN: JPCBFK; ISSN: 1520-6106
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We present a first-principles study of the structural, electronic, and optical properties of four conjugated polymers, poly(p-phenylene) (PPP), poly(2,7-fluorene) (PF), poly(2,7-carbazole) (PC), and poly(2,7-borafluorene) (PBF), and of their isolated constituent mols. All the calcns. were done using d.-functional theory (DFT) with a plane-wave basis set, pseudopotentials, and local exchange-correlation energy. Resemblances in the atomic structures of the systems studied allow us to make correspondences between their wave functions near the Fermi energy. The dihedral angles of the polymers under consideration are all similar, varying between 26° and 27°. In agreement with exptl. data, we find smaller energy gaps for carbazole and borafluorene compared to biphenyl and fluorene, which is due to differences in the HOMO or LUMO wave functions. However, for the polymers, the exptl. gap for PC was found to be almost the same as for PPP and PF. Our calcns. explain this exptl. observation which is attributed to a change in the ordering of the last two valence bands between carbazole and its polymer. We also find that the energy gap of PBF, which has not been synthesized yet, should be smaller than the min. energy gaps of the other studied polymers by .simeq.0.5 eV. The polarizations for the lowest electronic transitions are presented from the anal. of the wave functions' symmetries. We find excellent agreement between the calculated and available exptl. data, validating the predictions made.

IT 678974-54-4, Poly(5-methyl-5H-dibenzoborole-3,7-diyl) (electronic, structural, and optical properties of conjugated polymers based on carbazole, fluorene, and borafluorene)

RN 678974-54-4 HCAPLUS

CN Poly(5-methyl-5H-dibenzoborole-3,7-diyl) (9CI) (CA INDEX NAME)



CC 36-5 (Physical Properties of Synthetic High Polymers)
 Section cross-reference(s): 73

IT 92-52-4, Biphenyl, properties 1484-12-4 4569-45-3
 25190-62-9, Poly(1,4-phenylene) 678974-52-2,

Poly(9,9-dimethyl-9H-fluorene-2,7-diyl) 678974-53-3,
 Poly(9-methyl-9H-carbazole-2,7-diyl) 678974-54-4,
 Poly(5-methyl-5H-dibenzoborole-3,7-diyl) 678974-55-5

(electronic, structural, and optical properties of conjugated
 polymers based on carbazole, fluorene, and borafluorene)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

=> d 15 2-3 ibib abs hitstr hitind

L5 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:20737 HCAPLUS

DOCUMENT NUMBER: 140:84347

TITLE: Polymer and polymeric luminescent element
 comprising the same

INVENTOR(S): Tamao, Kohei; Yamaguchi, Shigehiro; Kitano,
 Makoto; Kobayashi, Satoshi; Sekine, Chizu

PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan;
 Kansai Technology Licensing Organization Co.,
 Ltd.

SOURCE: PCT Int. Appl., 87 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004003053	A1	20040108	WO 2003-JP8050	2003 0625
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004083548	A2	20040318	JP 2002-346790	2002 1129
AU 2003244054	A1	20040119	AU 2003-244054	2003 0625
JP 2004162011	A2	20040610	JP 2003-180646	2003 0625
US 2005170202	A1	20050804	US 2003-518713	2003 0625
PRIORITY APPLN. INFO.:			JP 2002-185712	A

2002
0626

JP 2002-281218

A

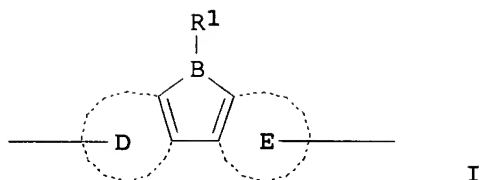
2002
0926

WO 2003-JP8050

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2003
0625

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AB The present invention relates to a polymer with no. average mol. weight 103-108 (based on polystyrene) comprising repeating units I, wherein R1 = H, alkyl, alkoxy, alkylthio, aryl, aryloxy, arylthio, arylalkyl, arylalkoxy, arylalkylthio, arylalkenyl, arylalkynyl, amino, substituted amino, silyl, substituted silyl, silyloxy, substituted silyloxy, monovalent heterocyclic group, or halogeno and D, E = (substituted) aromatic ring. Thus, 2.0 g 4,4'-dibromo-2,2'-diiodo-5,5'-dioctyloxy-1,1'-biphenyl (preparation given) 1.01 g (2,4,6-triisopropylphenyl)dimethoxyborane were reacted for 12 h to give 20.5 g 3,7-dibromo-5-(2,4,6-triisopropylphenyl)-2,8-dioctyloxy-5H-dibenzo[b, d]borole, 0.41 g of which was polymerized in the presence of 1.0 g bis(1,5-cyclooctadiene)nickel to give a copolymer with Mn 6.1 + 103 and Mw 9.9 + 103, which was spin-coated on a quartz to give a thin film giving a fluorescence peak at 564 nm.

IT 641629-37-0P

(preparation of luminescent polymers)

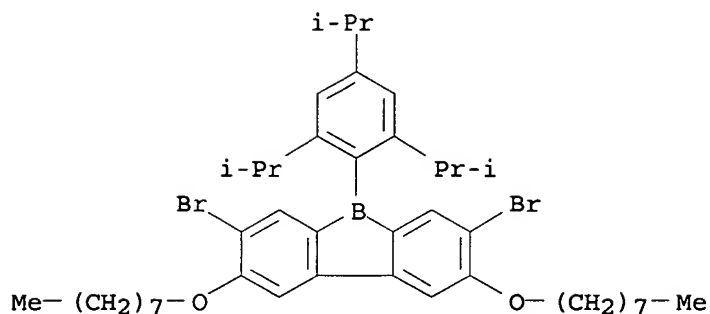
RN 641629-37-0 HCAPLUS

CN 5H-Dibenzoborole, 3,7-dibromo-2,8-bis(octyloxy)-5-[2,4,6-tris(1-methylethyl)phenyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 641629-36-9

CMF C43 H61 B Br2 O2



IC ICM C08G061-10
 ICS C08G061-12; H05B033-14; C09K011-06; C09D011-00
 CC 73-5 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
 Section cross-reference(s): 35, 38, 42
 IT 641629-37-0P
 (preparation of luminescent polymers)
 REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1970:465569 HCAPLUS
 DOCUMENT NUMBER: 73:65569
 TITLE: Azomethine derivatives. XI. Monomeric and dimeric arylmethyleamino- and diarylmethyleamino-boron compounds
 AUTHOR(S): Summerford, C.; Wade, Kenneth
 CORPORATE SOURCE: Chem. Dep., Durham Univ., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] A: Inorganic, Physical, Theoretical (1970), (12), 2010-16
 CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal
 LANGUAGE: English

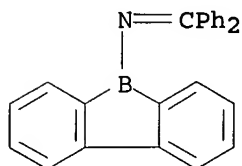
AB The monomeric aryl- and diarylmethyleaminoboranes Ph₂C:NBPh₂, (p-MeC₆H₄)₂C:NBPh₂, (p-ClC₆H₄)₂C:NBPh₂, p-BrC₆H₄PhC:NBPh₂, Ph₂C:NB(2,4,6-Me₃C₆H₂)₂, PhCH:NB(2,4,6-Me₃C₆H₂)₂, and QC:NBPh₂ (Q = 2,2'-biphenylene in this abstract) were prepared by one or more of the following routes: (1) R₁₂C:NSiMe₃ + R₂₂BX; (2) R₂₂C:LNi + R₂₂BX; (3) 2R₁₂C:NH + R₂₂BX; (4) R₁₂C:NBX₂ + 2R₂Li; (5) R₁₂C:NH₂ + Cl- + NaBPh₄ (X = halogen). The intermediate adduct (p-MeC₆H₄)₂C:NH, BPh₃ was isolated in a reaction of type 5. The associated alkylideneaminoboranes (Ph₂C:NBPhCl)_n, (PhCH:NBPhCl)₂, (PhCH:NBPh₂)₂, (Ph₂C:NBQ)_n, and (Ph₂C:NBO₂C₆H₄)_n were similarly prepared. The monomeric alkylideneaminoboranes are apparently prevented from dimerizing by the bulk of the substituents, especially on boron, which also inhibit approach of potential donor mols. Except for the air-stable Ph₂C:NB(C₆H₂Me₃-2,4,6)₂, they are hydrolyzed by moist air. Their ir spectra have characteristic absorptions, assigned ν(C : N .dblharw. B), in the range 1765-1820 cm⁻¹. ¹H NMR and mass spectra of the compds. are discussed.

IT 28499-73-2P
 (preparation of)
 RN 28499-73-2 HCAPLUS

CN 5H-Dibenzoborole, 5-[(diphenylmethylene)amino]-, polymers (8CI)
(CA INDEX NAME)

CM 1

CRN 47543-29-3
CMF C25 H18 B N



CC 22 (Physical Organic Chemistry)
IT 17814-66-3P 28499-73-2P 28499-93-6P 28499-94-7P
29097-39-0P 29097-40-3P 29097-41-4P 29098-26-8P
29098-27-9P 29098-28-0P
(preparation of)

=> d 112 1-77 ibib abs hitstr hitind

L12 ANSWER 1 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1031831 HCAPLUS
DOCUMENT NUMBER: 141:426346
TITLE: Non-aqueous electrolyte secondary battery
INVENTOR(S): Iwamoto, Kazuya; Koshina, Hizuru; Shimamura, Harunari; Nitta, Yoshiaki
PATENT ASSIGNEE(S): Matsushita Electric Industrial Co., Ltd., Japan
SOURCE: U.S., 14 pp., Cont.-in-part of U.S. 6,090,505.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6824920	B1	20041130	US 2000-601421	2000 0928
US 6090505	A	20000718	US 1998-90484	1998 0603
JP 2000173652	A2	20000623	JP 1998-342887	1998 1202
JP 2000173589	A2	20000623	JP 1998-342888	1998 1202

WO 2000033403

A1

20000608

WO 1999-JP6689

1999
1130

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W: US

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU,
MC, NL, PT, SE

PRIORITY APPLN. INFO.:

JP 1997-144873

A

1997
0603

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JP 1998-123199

A

1998
0506

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US 1998-90484

A2

1998
0603

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JP 1998-342887

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JP 1998-342888

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WO 1999-JP6689

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1999
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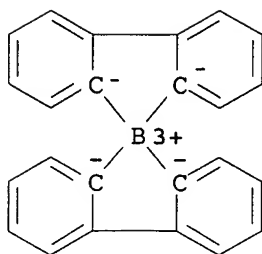
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AB A nonaq. electrolyte secondary battery consists of a cathode, an anode capable of intercalating and de-intercalating lithium, a non-aqueous electrolyte solution, and a separator or a solid electrolyte. The anode consists of composite particles made of tin, silicon or zinc coated with a solid solution or an intermetallic compound. The intermetallic compound contains Sn, Si, or Zn and an addnl. elements, such as Mg, Fe, Mo, Zn, Cd, In, Pb, Co, Ni, Al, Sn, Cu, V, or Ge. The electrolyte consists of a lithium salts of an organic acid dissolved in an organic solvent with high oxidation resistant characteristics. The lithium salts of an organic acid can be bistrifluoromethane sulfonic acid imido lithium, bis[1,2-benzenediolato(2-)-O,O'] lithium borate, bis[2,3-naphthalenediolato(2-)-O,O'] lithium borate, lithium bis(2,2'-biphenylene)borate, or bis(5-fluoro-2-olate-1-benzenesulfonic acid-O,O') lithium borate. The non-aqueous electrolyte can contain ethylene carbonate, di-Me carbonate, di-Et carbonate, ethylmethyl carbonate, propylene carbonate, γ -butyrolactone, or γ -valerolactone.

IT 108479-75-0, Lithium bis(2,2'-biphenylene)borate
(electrolyte; non-aqueous electrolyte secondary battery)

RN 108479-75-0 HCAPLUS

CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, lithium, (T-4)- (9CI)
(CA INDEX NAME)



● Li⁺

IC ICM H01M004-38
ICS H01M004-42
INCL 429218100; 429229000; 429231950
CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
IT 96-48-0, γ -Butyrolactone 96-49-1, Ethylene carbonate
105-58-8, Diethyl carbonate 108-29-2, γ -Valerolactone
108-32-7, Propylene carbonate 616-38-6, Dimethyl carbonate
623-53-0, Ethylmethyl carbonate 90076-65-6 108479-75-0
, Lithium bis(2,2'-biphenylene)borate 132843-44-8
156762-86-6 185433-68-5 201536-28-9
(electrolyte; non-aqueous electrolyte secondary battery)
REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

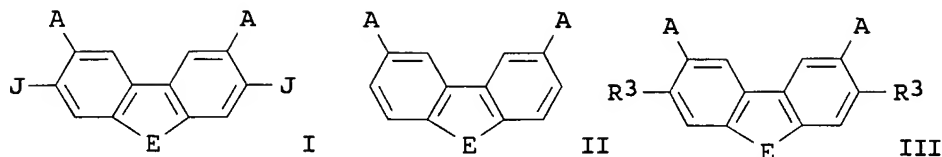
L12 ANSWER 2 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:559860 HCAPLUS
DOCUMENT NUMBER: 139:124832
TITLE: Functionalized 9-metalated fluorene
derivatives for organic electroluminescent
materials and their preparation
INVENTOR(S): Yamaguchi, Shigehiro; Tamao, Kohei
PATENT ASSIGNEE(S): Kansai Technology Licensing Organization Co.,
Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003206289	A2	20030722	JP 2002-51	2002 0104

PRIORITY APPLN. INFO.: JP 2002-51
2002
0104

OTHER SOURCE(S): MARPAT 139:124832

GI



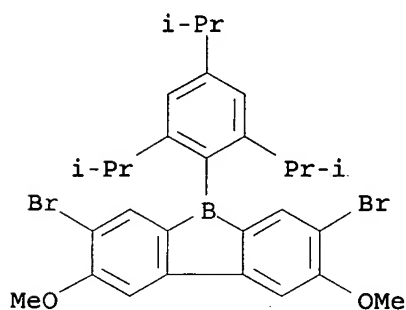
AB The derivs., having lower LUMO than that of fluorene, are I [A = ortho-inductive substituents, e.g., OR, NR₂, O(CH₂)_nOR, NR(CH₂)_nNR₂, etc. (R = C1-12 alkyl; n = 1-3); J = F-excluded halo, metal functional group; E = substituted Si or B], and are synthesized in high yield by these steps; halogenating 4 and 4' position of biphenyl derivs. II (A = the same as above), lithiating 2 and 2' position, and reacting with R₁R₂SiXY or R₁BXY (R₁, R₂ = C1-12 alkyl, aryl; X, Y = halo, alkoxy). The I may be prepared from II (A, E = the same as above) by lithiation at 2 and 7 position followed by reaction with electrophilic halogenating/metalating agents. Electroluminescent materials represented by III [A, E = the same as above; R₃ = aryl(vinyl), arylolethynyl, heteroaryl(vinyl), heteroarylolethynyl] are further claimed.

IT 454182-34-4P 454182-35-5P

(preparation of dibenzosilole or dibenzoborole derivs. for organic electroluminescent materials having lower LUMO than that of fluorenes)

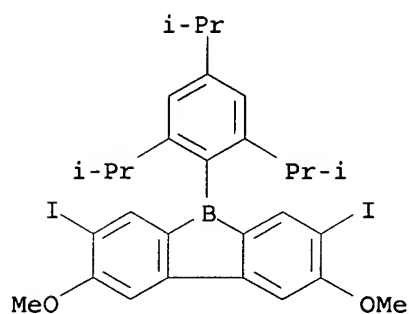
RN 454182-34-4 HCAPLUS

CN 5H-Dibenzoborole, 3,7-dibromo-2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 454182-35-5 HCAPLUS

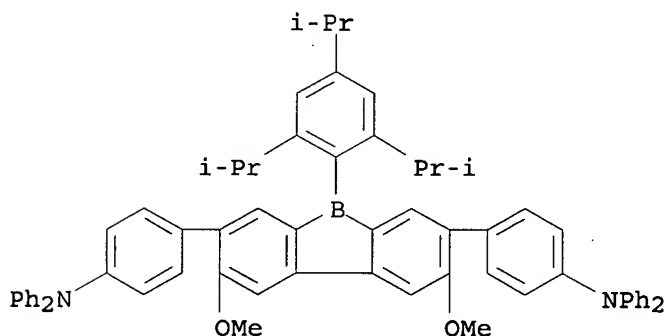
CN 5H-Dibenzoborole, 3,7-diiodo-2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



IT 454182-31-1P 454182-32-2P 454182-33-3P
 (preparation of dibenzosilole or dibenzoborole derivs. for organic electroluminescent materials having lower LUMO than that of fluorenes)

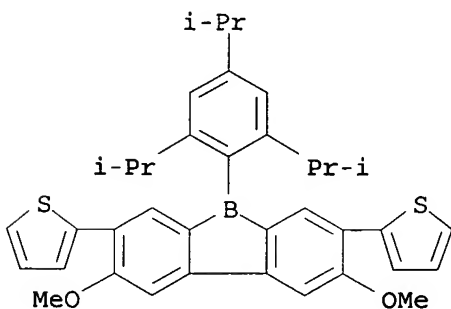
RN 454182-31-1 HCAPLUS

CN Benzenamine, 4,4'-[2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]-5H-dibenzoborole-3,7-diyl]bis[N,N-diphenyl- (9CI) (CA INDEX NAME)



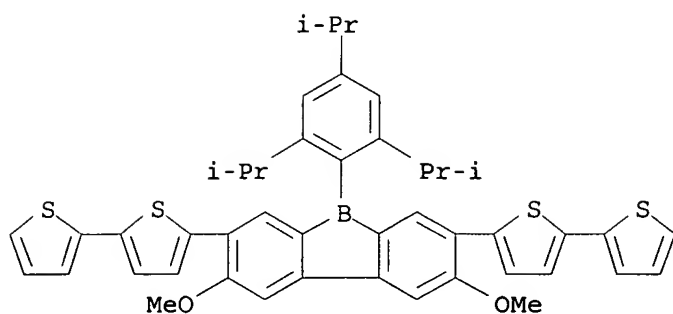
RN 454182-32-2 HCAPLUS

CN 5H-Dibenzoborole, 2,8-dimethoxy-3,7-di-2-thienyl-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 454182-33-3 HCAPLUS

CN 5H-Dibenzoborole, 3,7-bis([2,2'-bithiophen]-5-yl)-2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



IC ICM C07F005-02
ICS C07F007-08; C09K011-06
CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 29
IT 454182-34-4P 454182-35-5P 454182-36-6P
565225-98-1P 565226-00-8P 565226-02-0P
(preparation of dibenzosilole or dibenzoborole derivs. for organic electroluminescent materials having lower LUMO than that of fluorenes)
IT 454182-31-1P 454182-32-2P 454182-33-3P
565226-03-1P
(preparation of dibenzosilole or dibenzoborole derivs. for organic electroluminescent materials having lower LUMO than that of fluorenes)

L12 ANSWER 3 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:978639 HCAPLUS
DOCUMENT NUMBER: 138:39745
TITLE: Process for preparing maleic anhydride-modified polyolefins by oxidized adducts of borane and maleic anhydride
INVENTOR(S): Chung, Tze-Chiang
PATENT ASSIGNEE(S): Penn State Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 10 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002198327	A1	20021226	US 2002-156946	2002 0530
US 6699949	B2	20040302	US 2001-293977P	2001 0530

PRIORITY APPLN. INFO.: <--

AB The process comprises (a) mixing trialkylborane (e.g., tributylborane) with maleic anhydride and polyolefin (e.g., atactic polypropylene) in an inert organic solvent at 0-150°

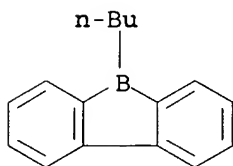
to form a reaction mixture containing a trialkylborane-maleic anhydride complex; (b) contacting the reaction mixture with an oxygen-containing oxidizing agent for 10 min-10 h at 0-150° at mole ratio of oxidizing agent to trialkylborane 1/2-4/3 to form a monooxidized trialkylborane adduct that undergoes hemolytic cleavage to form an alkoxy radical, wherein alkoxy radical, in turn, activates the chain of the polyolefin by alkoxy radical hydrogen-abstraction, and initiates an addition reaction between the maleic anhydride and the activated polyolefin to produce a modified polyolefin having maleic anhydride side groups; and (c) recovering the modified polyolefin. The maleic anhydride-modified polyolefin prepared has controlled mol. weight and maleic anhydride content.

IT 7760-71-6

(process of preparing maleic anhydride-modified polyolefins by oxidation adducts of borane and maleic anhydride)

RN 7760-71-6 HCAPLUS

CN 5H-Dibenzoborole, 5-butyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C08F255-00

INCL 525251000

CC 35-8 (Chemistry of Synthetic High Polymers)

IT 97-94-9, Triethylborane 280-64-8D, 9-Borabicyclononane, alkyl derivative 1069-54-1D, Disiamylborane, alkyl derivative 1116-61-6, Tripropylborane 1568-65-6D, Dicyclohexylborane, alkyl derivative 1883-38-1, Tripentylborane 3248-78-0, Trioctylborane 7397-46-8D, Methoxydiethylborane, adduct with maleic anhydride, oxidized 7760-71-6 51458-06-1D, Dimesitylborane, alkyl derivative 478917-44-1D, alkyl derivative (process of preparing maleic anhydride-modified polyolefins by oxidation adducts of borane and maleic anhydride)

L12 ANSWER 4 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:928599 HCAPLUS

DOCUMENT NUMBER: 138:303716

TITLE: syn-Sesquinorbornenyl carbocations and their boron analogues: an ab initio and DFT study

AUTHOR(S): Eckert-Maksic, Mirjana; Antol, Ivana; Margetic, Davor; Glasovac, Zoran

CORPORATE SOURCE: Division of Organic Chemistry and Biochemistry, Rudjer Boskovic Institute, Zagreb, HR-10002, Croatia

SOURCE: Journal of the Chemical Society, Perkin Transactions 2 (2002), (12), 2057-2063
CODEN: JCSPGI; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB MP2 and DFT calcns. employing 6-31G* were carried out to study the structure of some of the carbocations and their B analogs embedded in the syn-sesquinorbornene framework, hitherto not observed exptl. The calculated min. energy structures of all species provide evidence

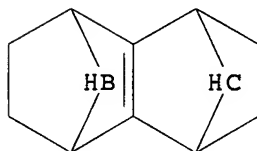
for homoconjugative interaction between the electron deficient center(s) and the C-C double bond. The use of isodesmic reactions based upon MP2(fc)/6-31G* energies indicates that the homoconjugative stabilization of mono- and di-cations is greater than those of the isoelectronic B compds. The calculated ^{13}C and ^{11}B NMR chemical shifts support this conclusion.

IT 507266-25-3

(ab initio and DFT study of syn-sesquinorbornenyl carbocations and their boron analogs)

RN 507266-25-3 HCAPLUS

CN 1,4-Borylene-5,8-methanonaphthalen-9-yl, 1,2,3,4,5,6,7,8-octahydro- (9CI) (CA INDEX NAME)



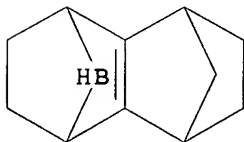
IT 507266-23-1 507266-24-2 507266-26-4

507266-27-5

(isodesmic hydride transfer; ab initio and DFT study of syn-sesquinorbornenyl carbocations and their boron analogs)

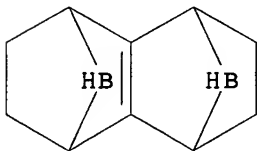
RN 507266-23-1 HCAPLUS

CN 1,4-Borylene-5,8-methanonaphthalene, 1,2,3,4,5,6,7,8-octahydro- (9CI) (CA INDEX NAME)



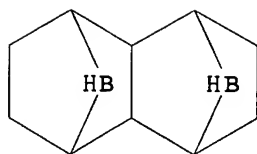
RN 507266-24-2 HCAPLUS

CN 1,4:5,8-Diborylenenaphthalene, 1,2,3,4,5,6,7,8-octahydro- (9CI) (CA INDEX NAME)

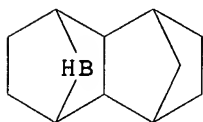


RN 507266-26-4 HCAPLUS

CN 1,4:5,8-Diborylenenaphthalene, decahydro- (9CI) (CA INDEX NAME)



RN 507266-27-5 HCAPLUS
 CN 1,4-Borylene-5,8-methanonaphthalene, decahydro- (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)
 IT 507266-22-0 507266-25-3
 (ab initio and DFT study of syn-sesquinorbornenyl carbocations and their boron analogs)
 IT 23010-44-8, Bicyclo[2.2.1]hept-2-en-7-ylum 32021-58-2
 143172-45-6, 7-Borabicyclo[2.2.1]hept-2-ene 507266-21-9
 507266-23-1 507266-24-2 507266-26-4
 507266-27-5 507444-50-0 507444-51-1
 (isodesmic hydride transfer; ab initio and DFT study of syn-sesquinorbornenyl carbocations and their boron analogs)
 REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2002:685440 HCAPLUS
 DOCUMENT NUMBER: 137:370137
 TITLE: The Theoretical Design of Neutral Planar Tetracoordinate Carbon Molecules with C(C)4 Substructures
 AUTHOR(S): Wang, Zhi-Xiang; Schleyer, Paul von Rague
 CORPORATE SOURCE: Computational Chemistry Annex, University of Georgia, Athens, GA, 30602-2525, USA
 SOURCE: Journal of the American Chemical Society (2002), 124(40), 11979-11982
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Using a new charge-compensation strategy, neutral mols. were designed with perfectly planar C(C)4-type tetracoordinate carbon arrangements (ptC) employing DFT computations. These designs, based on the planar preference of methane dications, replace two remote carbons in spiroalkaplanes by borons or two remote hydrogens by BH3 groups; the two formally anionic boron units which result compensate the formal double pos. charge on the central ptC's. The LUMOs correspond to the "wasted" lone pair HOMOs of the alkaplanes. As compared to the latter, π occupancies on the central carbon are much smaller (less than

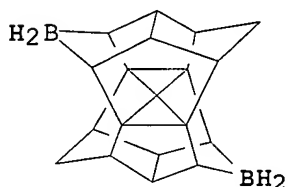
0.7e), and the IPs are much larger. The newly predicted compds. utilize all of the electrons more effectively. There are no lone pairs, and the ptC-C bond lengths are ca. 1.50 Å. The Wiberg bond index sums of the ptC's are near 3.2, and the boron sums are close to 4.

IT 475276-94-9

(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

RN 475276-94-9 HCAPLUS

CN 4,9,14,18-Methyno-1,20-dibora-1,2:16,20-diseco[5]fullerane-C20-Ih, 1,20-dihydro- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 24

IT 74-82-8, Methane, properties 157-40-4, Spiropentane 20741-88-2, Methane(1+), properties 73353-64-7, Indeno[7,1-cd]indene 101517-28-6, Spiro[2.2]pentane, radical ion(1+) 148810-14-4, Methane, radical ion(2+), properties 179032-57-6, Spiro[2.2]octaplane 251918-68-0 330597-93-8 475276-87-0 475276-88-1 475276-89-2 475276-90-5 475276-91-6 475276-92-7 475276-93-8 475276-94-9 475276-95-0 475276-96-1 475276-97-2 475276-98-3 475467-16-4 475467-22-2

(theor. study of tetracoordinate carbon mols. with C(C)4 substructures)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:624945 HCAPLUS

DOCUMENT NUMBER: 137:353357

TITLE: Boroxyl-based living free radical initiators

AUTHOR(S): Han, H.; Xu, G.; Chung, T. C.

CORPORATE SOURCE: Dep. Materials Sci. Eng., Pennsylvania State Univ., University Park, PA, 16802, USA

SOURCE: Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2002), 43(2), 82-83

CODEN: ACPPAY; ISSN: 0032-3934

PUBLISHER: American Chemical Society, Division of Polymer Chemistry

DOCUMENT TYPE: Journal; (computer optical disk)

LANGUAGE: English

AB Living radical polymerization occurring at ambient temperature with the injection of oxygen to 9-borofluorene derivs. in the presence of monomers was studied. The diminished chain-transfer and termination reactions in the homogeneous reaction conditions imply the in situ formation of a stable borinate radical, which serves as the reversible capping agent with the propagating radical

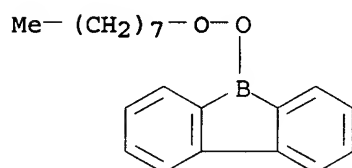
during the living radical polymerization The functionalization of polyolefins occurred by first incorporating borane groups into the polyolefin chain that were then spontaneously monooxidized by oxygen to form peroxide (B-O-O-C) moieties. Next, these moieties initiated free radical graft-from polymerization of functional monomers (such as acrylic and methacrylic monomers) at ambient temperature to form polyolefin graft and block copolymers containing polyolefin and functional polymer segments. Ethylene-Me methacrylate block copolymers and PMMA were prepared using this method. and were white solids with well-defined mol. structures.

IT 441019-27-8P

(boroxyl-based living free radical initiator for polymerization of vinyl compds. and polymerization mechanism)

RN 441019-27-8 HCAPLUS

CN 5H-Dibenzoborole, 5-(octyldioxy)- (9CI) (CA INDEX NAME)

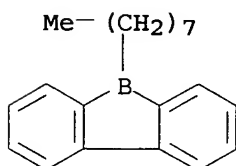


IT 441019-26-7

(oxidation of; boroxyl-based living free radical initiator for polymerization of vinyl compds. and polymerization mechanism)

RN 441019-26-7 HCAPLUS

CN 5H-Dibenzoborole, 5-octyl- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

IT 441019-27-8P

(boroxyl-based living free radical initiator for polymerization of vinyl compds. and polymerization mechanism)

IT 441019-26-7

(oxidation of; boroxyl-based living free radical initiator for polymerization of vinyl compds. and polymerization mechanism)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:522666 HCAPLUS

DOCUMENT NUMBER: 137:94184

TITLE: Alkylperoxydiarylborane derivatives as initiators for living free radical polymerization

INVENTOR(S): Chung, Tze-chiang

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 17 pp.

DOCUMENT TYPE: CODEN: USXXCO
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: English
 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002091211	A1	20020711	US 2001-887116	2001 0625
US 6420502	B2	20020716	<--	
US 2002198338	A1	20021226	US 2002-156945	2002 0530
US 6515088	B2	20030204	<--	
PRIORITY APPLN. INFO.:			US 2000-242592P	P 2000 1023
			<--	
			US 2001-887116	A3 2001 0625
			<--	

OTHER SOURCE(S): MARPAT 137:94184

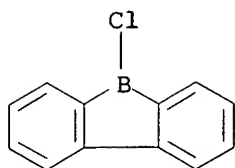
AB New living free radical initiators are based on alkylperoxydiarylborane and its derivs. that may be represented by the general formula $R-[O-O-B-Ph_1(Ph_2)]_n$ where n is from 1 to 4, R is a hydrogen or a linear, branched or cyclic alkyl radical having a mol. weight from 1 to about 500, and Ph1 and Ph2 are independently selected from aryl radicals, based on Ph or substituted Ph groups, with the proviso that Ph1 and Ph2 can be the chemical bridged to each other with a linking group or with a direct chemical bond between the two aryl groups to form a cyclic ring structure that includes a boron atom. At ambient temperature the $R-[O-O-B-Ph_1(Ph_2)]_n$ species spontaneously homolyzes to form an alkoxyl radical $R-[O\cdot]_n$, which is active in initiating living polymerization of polymerizable monomers, and a dormant diarylborinate radical $\cdot O-B-Ph_1(Ph_2)$, which is too stable to initiate polymerization due to the back-donating of electron d. to the empty p-orbital of boron, but which may form a reversible bond with the radical at the growing polymer chain end to prevent undesirable side reactions. Thus, 1-octylperoxy-9-borafluorene initiator was synthesized and used in radical polymerization of MMA and Bu methacrylate. The polymns. were living as indicated by a linear increase of polymer mol. weight with monomer conversion, a narrow mol. weight distribution, and the formation of block copolymers by sequential monomer addition

IT 13059-59-1P, 9-Chloro-9-borafluorene 14265-95-3P
 , Bis(9-borafluorene) 441019-26-7P

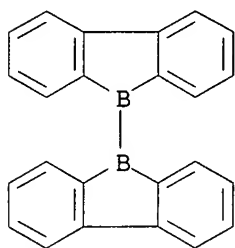
(in synthesis of initiators based on alkylperoxydiarylborane derivs. for living free radical polymerization)

RN 13059-59-1 HCAPLUS

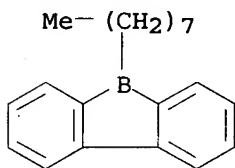
CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



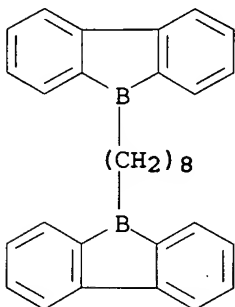
RN 14265-95-3 HCAPLUS
 CN 5,5'-Bi-5H-dibenzoborole (8CI, 9CI) (CA INDEX NAME)



RN 441019-26-7 HCAPLUS
 CN 5H-Dibenzoborole, 5-octyl- (9CI) (CA INDEX NAME)

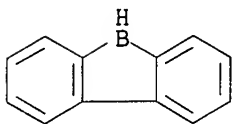


IT 441019-28-9P
 (in synthesis of initiators based on alkylperoxydiarylborane
 derivs. for living free radical polymerization)
 RN 441019-28-9 HCAPLUS
 CN 5H-Dibenzoborole, 5,5'-(1,8-octanediyl)bis- (9CI) (CA INDEX NAME)

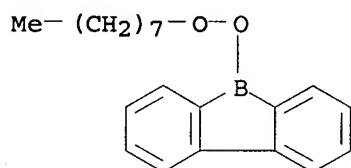


IT 244-33-7, 9-Borafluorene
 (in synthesis of initiators based on alkylperoxydiarylborane
 derivs. for living free radical polymerization)
 RN 244-33-7 HCAPLUS

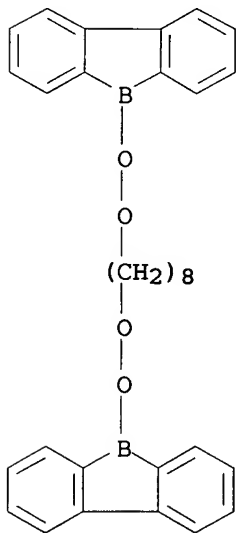
CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 441019-27-8P 441019-29-0P
 (initiators based on alkylperoxydiarylborane derivs. for living
 free radical polymerization)
 RN 441019-27-8 HCAPLUS
 CN 5H-Dibenzoborole, 5-(octyldioxy)- (9CI) (CA INDEX NAME)



RN 441019-29-0 HCAPLUS
 CN 5H-Dibenzoborole, 5,5'-[1,8-octanediylbis(dioxy)]bis- (9CI) (CA
 INDEX NAME)



IC ICM C08F004-12
 INCL 526196000
 CC 35-3 (Chemistry of Synthetic High Polymers)
 IT 13029-09-9P, 2,2'-Dibromobiphenyl 13059-59-1P,
 9-Chloro-9-borafluorene 14265-95-3P, Bis(9-borafluorene)
 441019-26-7P
 (in synthesis of initiators based on alkylperoxydiarylborane
 derivs. for living free radical polymerization)
 IT 16291-32-0P, 2,2'-Dilithiobiphenyl 441019-28-9P

(in synthesis of initiators based on alkylperoxydiarylborane derivs. for living free radical polymerization)

IT 111-66-0, 1-Octene 244-33-7, 9-Borafluorene 583-53-9,
o-Dibromobenzene 3710-30-3, 1,7-Octadiene 10294-34-5, Boron trichloride

(in synthesis of initiators based on alkylperoxydiarylborane derivs. for living free radical polymerization)

IT 441019-27-8P 441019-29-0P
(initiators based on alkylperoxydiarylborane derivs. for living free radical polymerization)

L12 ANSWER 8 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:511736 HCAPLUS

DOCUMENT NUMBER: 137:201358

TITLE: Dibenzoborole-Containing π -Electron Systems: Remarkable Fluorescence Change Based on the "On/Off" Control of the $p\pi-\pi^*$ Conjugation

AUTHOR(S): Yamaguchi, Shigehiro; Shirasaka, Toshiaki; Akiyama, Seiji; Tamao, Kohei

CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Uji, Kyoto, 611-0011, Japan

SOURCE: Journal of the American Chemical Society (2002), 124(30), 8816-8817
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

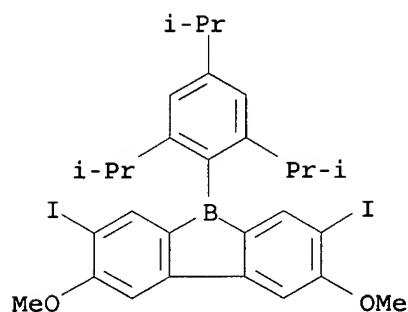
OTHER SOURCE(S): CASREACT 137:201358

AB Dibenzoborole derivs. with various groups such as (N,N-diphenylamino)phenyl, thienyl, and bithienyl groups at the 3,7-positions were synthesized and their photophys. properties studied. These new π -electron systems show significant solvatochromism in the fluorescence spectra. Thus, .apprx.100-140 nm blue shifts in the emission maxima and 20-30-fold increments in the quantum yields are observed upon changing the solvent from THF to DMF. Similar fluorescence changes are observed upon the addition of Bu₄NF to their THF solns., demonstrating their sensing abilities toward a fluoride ion. These fluorescence changes result from the on/off control of the $p\pi-\pi^*$ conjugation in their LUMO by the coordination of donor solvents or F⁻ ion to the B atom in the dibenzoborole skeleton.

IT 454182-35-5P
(preparation and Kosugi-Migita-Stille coupling reaction of, with arylstannanes in presence of palladium catalyst)

RN 454182-35-5 HCAPLUS

CN 5H-Dibenzoborole, 3,7-diiodo-2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

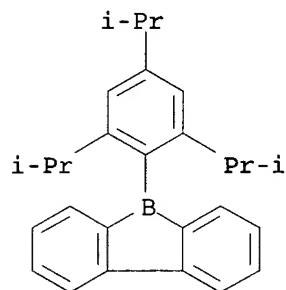


IT 454182-30-0P

(preparation and fluorescence of)

RN 454182-30-0 HCAPLUS

CN 5H-Dibenzoborole, 5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

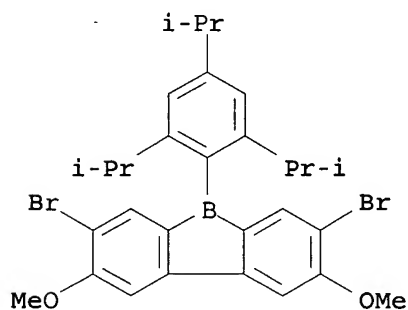


IT 454182-34-4P

(preparation and iodination of)

RN 454182-34-4 HCAPLUS

CN 5H-Dibenzoborole, 3,7-dibromo-2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

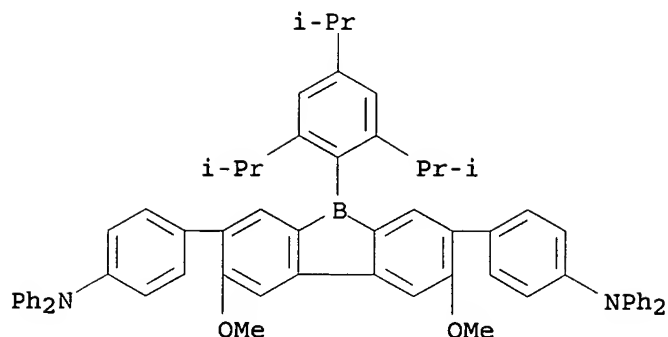


IT 454182-31-1P 454182-32-2P 454182-33-3P

(solvatochromism; preparation and changes in fluorescence spectrum upon coordination of donor solvents or fluoride ion)

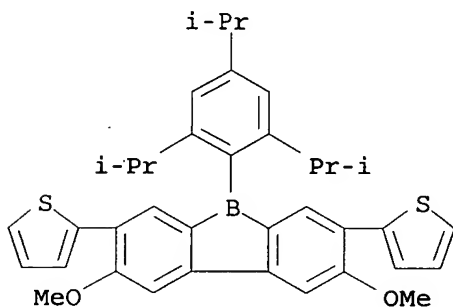
RN 454182-31-1 HCAPLUS

CN Benzenamine, 4,4'-[2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]-5H-dibenzoborole-3,7-diyl]bis[N,N-diphenyl]- (9CI) (CA INDEX NAME)



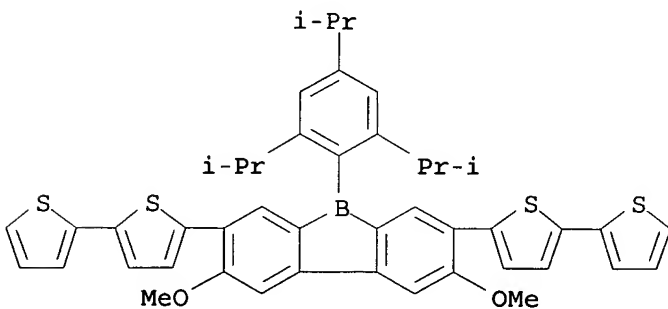
RN 454182-32-2 HCAPLUS

CN 5H-Dibenzoborole, 2,8-dimethoxy-3,7-di-2-thienyl-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 454182-33-3 HCAPLUS

CN 5H-Dibenzoborole, 3,7-bis([2,2'-bithiophen]-5-yl)-2,8-dimethoxy-5-[2,4,6-tris(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 73

IT 454182-35-5P

(preparation and Kosugi-Migita-Stille coupling reaction of, with arylstannanes in presence of palladium catalyst)

IT 454182-30-0P

(preparation and fluorescence of)

IT 454182-34-4P

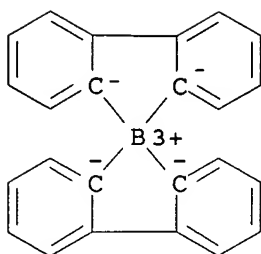
(preparation and iodination of)
IT 454182-31-1P 454182-32-2P 454182-33-3P
(solvatochromism; preparation and changes in fluorescence spectrum
upon coordination of donor solvents or fluoride ion)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L12 ANSWER 9 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:292085 HCAPLUS
DOCUMENT NUMBER: 136:332792
TITLE: IR laser heat mode type negative working
lithographic printing plate master
INVENTOR(S): Shimada, Kazuto; Nakamura, Ippei; Sorori,
Tadahiro
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2002116539	A2	20020419	JP 2000-310808	2000 1011

PRIORITY APPLN. INFO.: <-- JP 2000-310808
2000
1011

OTHER SOURCE(S): MARPAT 136:332792
AB The title heat mode type neg. working lithog. printing plate
master contains (A) an onium type polymerization initiator, (B) a
photothermal conversion compound, (C) a polymerizable compound, and
(D) a borate compound represented by Ar₄B-M⁺ (M⁺ = cation; Ar =
aromatic) in a photosensitive layer. The printing plate master shows
excellent sensitivity and storage stability.
IT 108479-75-0
(borate compound in photosensitive layer of IR laser heat mode
type neg. working lithog. printing plate master to improve
sensitivity as well as storage stability)
RN 108479-75-0 HCAPLUS
CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, lithium, (T-4)- (9CI)
(CA INDEX NAME)



● Li⁺

IC ICM G03F007-029
ICS B41N001-14; G03F007-00; G03F007-004; G03F007-027

CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 143-66-8 15522-59-5 15525-15-2 26985-34-2
108479-75-0 144699-38-7 146761-08-2 153347-65-0
159123-85-0 412267-88-0 412267-90-4 412267-92-6
412267-93-7 412267-95-9 412267-96-0
(borate compound in photosensitive layer of IR laser heat mode type neg. working lithog. printing plate master to improve sensitivity as well as storage stability)

L12 ANSWER 10 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:614710 HCAPLUS

DOCUMENT NUMBER: 135:344537

TITLE: Heterobuckybowls: A Theoretical Study on the Structure, Bowl-to-Bowl Inversion Barrier, Bond Length Alternation, Structure-Inversion Barrier Relationship, Stability, and Synthetic Feasibility

AUTHOR(S): Priyakumar, U. Deva; Sastry, G. Narahari

CORPORATE SOURCE: Department of Chemistry, Pondicherry University, Pondicherry, 605 014, India

SOURCE: Journal of Organic Chemistry (2001), 66(20), 6523-6530
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hybrid d. functional theory (DFT) calcns. at the B3LYP/cc-pVDZ level were performed on a series of heterobuckybowls, 3X, C18X3H6 (X = O, NH, CH2, BH, S, PH, PH3, Si, SiH2, and AlH). The min. energy conformations and the transition states for bowl-to-bowl inversion, where the geometry is bowl shaped, are computed and characterized by frequency calcns. The geometries of heterotrindenes, 2X, C12X3H6 (X = O, NH, CH2, BH, S, PH, PH3, Si, SiH2, and AlH), were obtained, and the bond length alternation (Δ) in the central benzenoid ring shows remarkable sensitivity as a function of substituent with a wide range of fluctuations (-0.014 to +0.092 Å). The Δ computed in 2BH was found to be comparable with the highest bond alternation reported to date in benzenoid frameworks. The inversion dynamics of these heterobowls and their bowl depths were fit to a mixed

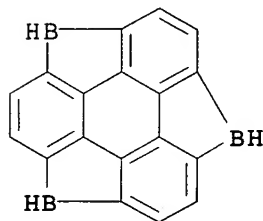
quartic/quadratic function. The size of the heteroatom seems to exclusively control the bowl depth and rigidity as well as the synthetic feasibility. In contrast, the bond length alternation seems to be controlled by electronic factors and not by the size of the substituted atom either in trindenenes or in heterosumanenes. The thermodyn. stability of this class of compds. is very much comparable with trithiasumanene (3S), which was synthesized recently. The chemical hardness (η) was measured to assess the stability of the heterosumanenes. The strain energy buildup in a sequential ring closure strategy along two synthetic routes, namely a triphenylene route and a trindene route, were explored, and the trindene route was found to be highly favorable for making such compds. compared to the triphenylene route. However, in both routes the ease of the synthetic feasibility increases as the size of the heteroatom increases.

IT 371785-58-9

(theor. study on structure, bowl-to-bowl inversion barrier, bond length alternation, structure-inversion barrier relationship, stability, and synthetic feasibility of heterobuckybowls)

RN 371785-58-9 HCAPLUS

CN 1H-Triphenyleno[1,12-bcd:4,5-b'c'd':8,9-b''c''d'']trisborole, 4,7-dihydro- (9CI) (CA INDEX NAME)

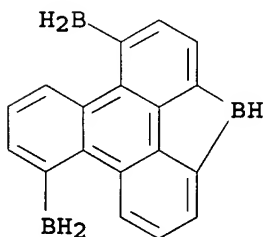


IT 371785-66-9 371785-75-0 371786-03-7

(theor. study on structure, bowl-to-bowl inversion barrier, bond length alternation, structure-inversion barrier relationship, stability, and synthetic feasibility of heterobuckybowls)

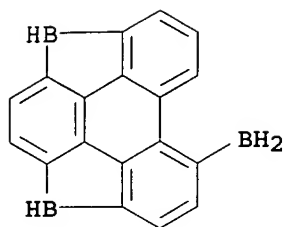
RN 371785-66-9 HCAPLUS

CN 4H-Triphenyleno[1,12-bcd]borole, 1,8-diboryl- (9CI) (CA INDEX NAME)

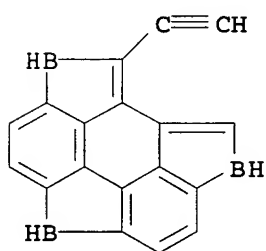


RN 371785-75-0 HCAPLUS

CN Triphenyleno[1,12-bcd:4,5-b'c'd']bisborole, 6-boryl-3,10-dihydro- (9CI) (CA INDEX NAME)



RN 371786-03-7 HCAPLUS
 CN 1H-Phenanthro[1,10-bc:4,5-b'c'd':8,9-b''c'']trisborole,
 5-ethynyl-4,7-dihydro- (9CI) (CA INDEX NAME)



CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22
 IT 151253-59-7 251991-63-6 260353-02-4 330163-77-4
 330163-78-5 371785-58-9 371785-59-0 371785-60-3
 371785-61-4 371785-62-5
 (theor. study on structure, bowl-to-bowl inversion barrier,
 bond length alternation, structure-inversion barrier
 relationship, stability, and synthetic feasibility of
 heterobuckybowls)
 IT 151253-57-5 151253-58-6 371785-64-7, Triphenyleno[1,12-
 bcd]furan-1,8-diol 371785-65-8 371785-66-9
 371785-67-0 371785-68-1 371785-69-2 371785-70-5
 371785-71-6 371785-72-7 371785-73-8 371785-74-9
 371785-75-0 371785-76-1 371785-77-2 371785-78-3
 371785-79-4 371785-80-7 371785-81-8 371785-90-9
 371785-91-0 371785-92-1 371785-93-2 371785-94-3
 371785-95-4 371785-96-5 371785-97-6 371785-98-7
 371785-99-8 371786-00-4 371786-01-5 371786-02-6
 371786-03-7 371786-04-8 371786-05-9 371786-06-0
 371786-07-1 371786-08-2 371786-09-3
 (theor. study on structure, bowl-to-bowl inversion barrier,
 bond length alternation, structure-inversion barrier
 relationship, stability, and synthetic feasibility of
 heterobuckybowls)
 REFERENCE COUNT: 92 THERE ARE 92 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L12 ANSWER 11 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:351869 HCAPLUS
 DOCUMENT NUMBER: 135:166540
 TITLE: Tailoring the curvature, bowl rigidity and
 stability of heterobuckybowls: theoretical

design of synthetic strategies towards heterosumanenes

AUTHOR(S): Priyakumar, U. D.; Sastry, G. N.

CORPORATE SOURCE: Department of Chemistry, Pondicherry University, Pondicherry, India

SOURCE: Journal of Molecular Graphics & Modelling (2001), 19(2), 266-269
CODEN: JMGMFI; ISSN: 1093-3263

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

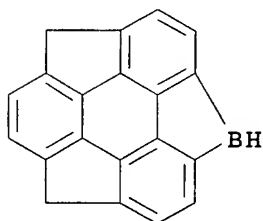
LANGUAGE: English

AB Quantum mech. calcns. predict that larger heteroatom substituents on the periphery increase the feasibility of the crucial third ring closure in sumanene and are responsible for the accompanying modulations in the curvature, rigidity, stability and some of the physicochem. properties of the resulting heterosumanenes. Systematic application of semiempirical, ab initio, and DFT methods reveal that the qual. trends obtained and our principal conclusions are independent of level of theory, albeit with minor quant. differences.

IT 353739-74-9
(strain energy; theor. design of synthetic strategies towards heterosumanenes)

RN 353739-74-9 HCAPLUS

CN 1H-Dicyclopenta[4,5:8,9]triphenylene[1,12-bcd]borole, 4,7-dihydro-(9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)
Section cross-reference(s): 29, 65

IT 151253-59-7, Sumanene 334541-89-8 353739-72-7 353739-73-8
353739-74-9 353739-75-0 353739-76-1 353739-77-2
353739-78-3
(strain energy; theor. design of synthetic strategies towards heterosumanenes)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:288498 HCAPLUS

DOCUMENT NUMBER: 135:76914

TITLE: BN-Doped Fullerenes: An NICS Characterization

AUTHOR(S): Chen, Zhongfang; Jiao, Haijun; Hirsch, Andreas; Thiel, Walter

CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Erlangen-Nuernberg, Erlangen, 91054, Germany

SOURCE: Journal of Organic Chemistry (2001), 66(10), 3380-3383
CODEN: JOCEAH; ISSN: 0022-3263

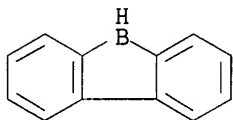
PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Heterofullerenes C58(BN), C54(BN)3, C48(BN)6, and C12(BN)24 and their hexaanions as well as the C58(BN) dimer were studied by ab initio calcns. From the computed nucleus independent chemical shifts (NICS) at the cage center and also at the center of individual rings, BN-doped fullerenes C58(BN), C54(BN)3, and C48(BN)6 are slightly more aromatic than C60, whereas the corresponding hexaanions are significantly less aromatic than C606-. The predicted NICS values may be useful for the identification of the heterofullerenes through their endohedral 3He NMR chemical shifts. Compared to C60, the dimerization of C58(BN) is more exothermic by 16 kcal/mol.

IT 244-33-7, 9-Borafluorene 347358-07-0,
 5H-Dibenzoborol-5-amine 347358-08-1
 (calcn. of NICS values at cage center of)

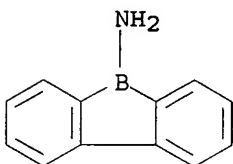
RN 244-33-7 HCAPLUS

CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



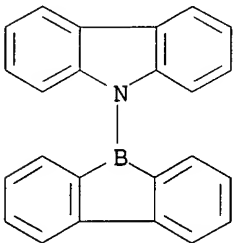
RN 347358-07-0 HCAPLUS

CN 5H-Dibenzoborol-5-amine (9CI) (CA INDEX NAME)



RN 347358-08-1 HCAPLUS

CN 9H-Carbazole, 9-(5H-dibenzoborol-5-yl)- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 86-74-8, 9-Azafluorene 91-20-3, Naphthalene, properties
 109-97-7, Pyrrole 187-78-0, Cyclopent[fg]acenaphthylene
 244-33-7, 9-Borafluorene 287-87-6, Borole 1425-58-7,

10,9-Borazaronaphthalene 45376-40-7 99685-96-8, C60 Fullerene
 139703-76-7, [5,6]Fulleride(6-)-C60-Ih 155472-06-3,
 1H-Borol-1-amine 155774-88-2, Fullerene-C120 192522-25-1
 347358-06-9 347358-07-0, 5H-Dibenzoborol-5-amine
 347358-08-1 347358-09-2

(calcn. of NICS values at cage center of)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

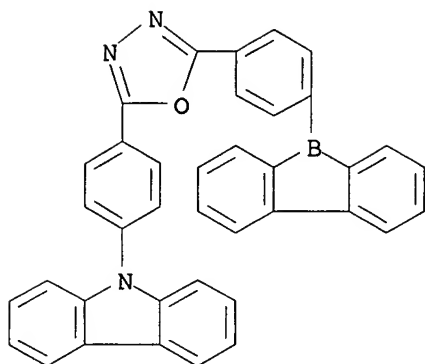
L12 ANSWER 13 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:242953 HCAPLUS
 DOCUMENT NUMBER: 134:287602
 TITLE: Organic electroluminescent component
 INVENTOR(S): Ueda, Noriko; Okubo, Yasushi; Kita, Hiroshi
 PATENT ASSIGNEE(S): Konica Co., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001093670	A2	20010406	JP 1999-274848	1999 0928

PRIORITY APPLN. INFO.: JP 1999-274848
 1999
 0928

OTHER SOURCE(S): MARPAT 134:287602
 AB The invention refers to an organic electroluminescent component
 containing at least one compound R1R2N(Q1)n1BAr1Ar2 [Ar1,2 =
 (un)substituted aryl, and may be joined to form a ring with the B
 atom; R1,2 = functional group, and may be joined to form a ring
 with the N atom; Q1 = (un)substituted arylene; n1 = 0 or 1].
 IT 332350-45-5
 (organic electroluminescent component)
 RN 332350-45-5 HCAPLUS
 CN 9H-Carbazole, 9-[4-[5-[4-(5H-dibenzoborol-5-yl)phenyl]-1,3,4-
 oxadiazol-2-yl]phenyl]- (9CI) (CA INDEX NAME)



IC ICM H05B033-14
ICS C09K011-06; H05B033-22
CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
IT 38186-32-2 38186-34-4 332350-25-1 332350-29-5 332350-31-9
332350-33-1 332350-35-3 332350-37-5 332350-39-7
332350-41-1 332350-42-2 332350-43-3 332350-44-4
332350-45-5 332350-46-6 332350-47-7 332350-48-8
332350-49-9 332350-50-2 332350-51-3 332350-52-4
332350-53-5 332350-54-6 332350-55-7 332350-56-8
(organic electroluminescent component)

L12 ANSWER 14 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:68588 HCAPLUS
DOCUMENT NUMBER: 134:280890
TITLE: Synthesis and Characterization of a Sterically Encumbered Unsymmetrical 9-Borfluorene, Its Pyridine Adduct, and Its Dilithium Salt
AUTHOR(S): Wehmschulte, Rudolf J.; Khan, Masood A.; Twamley, Brendan; Schiemenz, Berthold
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK, 73019, USA
SOURCE: Organometallics (2001), 20(5), 844-849
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:280890

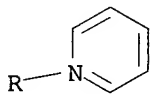
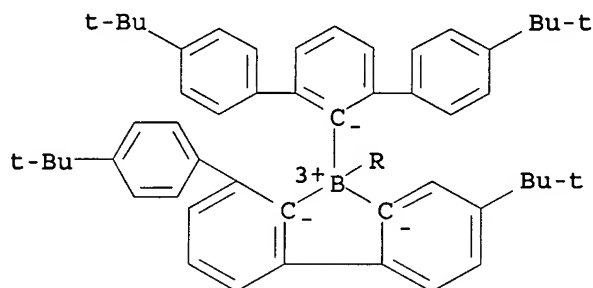
AB The reaction of 2,6-(4-*t*-BuC₆H₄)₂C₆H₃Li with [BH₂Cl.SMe₂] in hexane or Et₂O solution affords the terphenyl-substituted unsym. 9-borfluorene, 1-(4-*tert*-Butylphenyl)-7-*tert*-butyl-9-[2,6-bis(4-*tert*-butylphenyl)phenyl]-9-borfluorene (1), in good to moderate yields. Addition of pyridine gives the colorless crystalline adduct 1.py. Compound 1 is readily reduced to the deep red heteroarom. dianionic (μ -2- η 5, η 5-1-(4-*tert*-butylphenyl)-7-*tert*-butyl-9-[2,6-bis(4-*tert*-butylphenyl)phenyl]-9-borfluorenyl)bis(Et₂O)dilithium (2) with excess Li powder in Et₂O solution. Reactions of the dianionic 2 with various metal salts leads to reduction of these salts, and bright yellow 1 is recovered in essentially quant. yields. Compds. 1, 1.py, and 2 were characterized by ¹H, ¹³C, and ¹¹B NMR spectroscopy and compds. 1.py and 2 also by single-crystal x-ray diffraction.

IT 332104-79-7P 332104-81-1P
(preparation and crystal structure of)

RN 332104-79-7 HCAPLUS
 CN Boron, [4,4''-bis(1,1-dimethylethyl) [1,1':3',1''-terphenyl]-2,2'-diyl] [4,4''-bis(1,1-dimethylethyl) [1,1':3',1''-terphenyl]-2'-yl] (pyridine)-, (T-4)-, compd. with hexane (8:1) (9CI) (CA INDEX NAME)

CM 1

CRN 332104-78-6
 CMF C57 H62 B N
 CCI CCS



CM 2

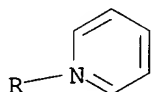
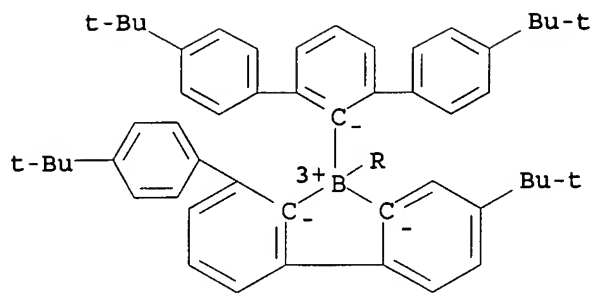
CRN 110-54-3
 CMF C6 H14

Me- (CH₂)₄-Me

RN 332104-81-1 HCAPLUS
 CN Boron, [4,4''-bis(1,1-dimethylethyl) [1,1':3',1''-terphenyl]-2,2'-diyl] [4,4''-bis(1,1-dimethylethyl) [1,1':3',1''-terphenyl]-2'-yl] (pyridine)-, (T-4)-, compd. with hexane (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 332104-78-6
 CMF C57 H62 B N
 CCI CCS



CM 2

CRN 110-54-3

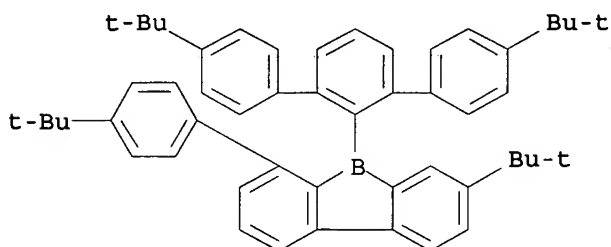
CMF C6 H14

$$\text{Me}-(\text{CH}_2)_4-\text{Me}$$

IT 332104-77-5P, 1-(4-tert-Butylphenyl)-7-tert-butyl-9-[2,6-bis(4-tert-butylphenyl)phenyl]-9-borafluorene
(preparation and reduction to heteroarom. dianionic derivative)

RN 332104-77-5 HCAPLUS

CN 5H-Dibenzoborole, 5-[4,4''-bis(1,1-dimethylethyl)[1,1':3',1''-terphenyl]-2'-yl]-3-(1,1-dimethylethyl)-6-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



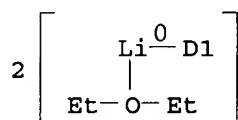
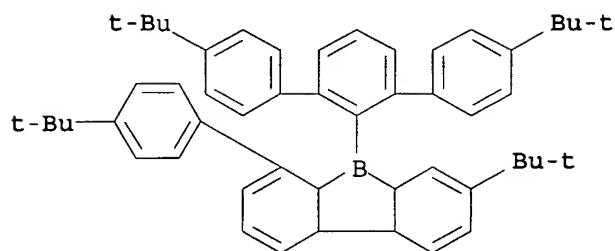
IT 332342-55-9P
(preparation, crystal structure, and reaction with metal salts)

RN 332342-55-9 HCAPLUS

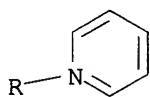
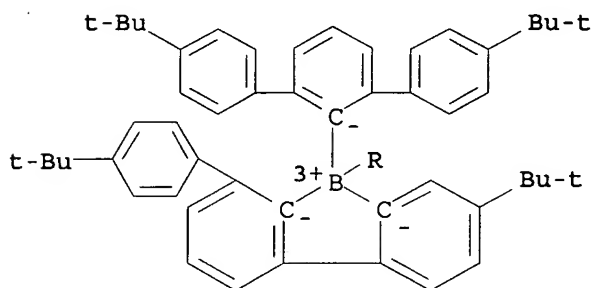
CN Lithium, [μ-[5-[4,4''-bis(1,1-dimethylethyl)[1,1':3',1''-terphenyl]-2'-yl]-3-(1,1-dimethylethyl)-6-[4-(1,1-dimethylethyl)phenyl]-5H-dibenzoborolodiyl]]bis[1,1'-oxybis[ethane]]di- (9CI) (CA INDEX NAME)

CM 1

CRN 332342-54-8
 CMF C60 H79 B Li2 O2
 CCI CCS, IDS



IT 332104-78-6P
 (preparation, mol. structure, and dissociation constant for loss of
 pyridine from)
 RN 332104-78-6 HCAPLUS
 CN Boron, [4,4''-bis(1,1-dimethylethyl) [1,1':3',1''-terphenyl]-2,2'-
 diyl] [4,4''-bis(1,1-dimethylethyl) [1,1':3',1''-terphenyl]-2'-
 yl] (pyridine)-, (T-4)- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 IT 332104-79-7P 332104-81-1P
 (preparation and crystal structure of)
 IT 332104-77-5P, 1-(4-tert-Butylphenyl)-7-tert-butyl-9-[2,6-
 bis(4-tert-butylphenyl)phenyl]-9-borfluorene
 (preparation and reduction to heteroarom. dianionic derivative)
 IT 332342-55-9P
 (preparation, crystal structure, and reaction with metal salts)

IT 332104-78-6P

(preparation, mol. structure, and dissociation constant for loss of pyridine from)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L12 ANSWER 15 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:37486 HCAPLUS

DOCUMENT NUMBER: 134:187473

TITLE: Hydridoborates and hydridoborato metallates
part 26. Preparation and structures of
dihydridoborates of lithium and potassium

AUTHOR(S): Knizek, Jorg; Noth, Heinrich

CORPORATE SOURCE: Department of Chemistry, Inorganic Chemistry,
University of Munich, Munich, D-81377, Germany

SOURCE: Journal of Organometallic Chemistry (2000),
614-615, 168-187

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

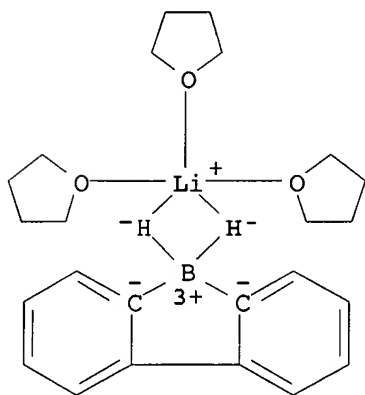
LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:187473

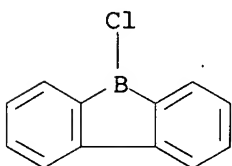
AB Alkali metal dihydrido borates were prepared by three different routes. They were characterized by ¹¹B-NMR spectroscopy and, in part, by IR spectroscopy. The following compds. were obtained: lithium dihydridodimethylborate and lithium methyltrihydridoborate, (1) and (2), lithium and potassium dihydridodi(tert-butyl)borate, (3) and (4), lithium dihydridodi(cyclopentyl)borate (5), lithium and potassium dihydrido(9-boratabicyclo[3.3.0]nonane), (6a,b), potassium dihydrido(boratacyclohexane) (7), lithium dihydridoboratacycloheptane (8), and lithium dihydrido-9-boratafluorene (9). In the process of the formation of 1 and 7 also Li(H₃BMe) (2) and Li₂(H₃B-(CH₂)₅-BH₃) are formed, most likely by a ligand redistribution process which is not operative if bulky organyl groups are bound to the boron atom or if the boron atom is part of a ring system. In case of catecholate no H₂B(OR)₂⁻ anions were detected but for ephedrino or dithiolato ligands the corresponding dihydrido borate complexes were readily detected by ¹¹B-NMR but the latter converted in THF solution into B(S₂R')₂ anions. MO calcns. show that the ligand redistribution for H₂BX₂⁻ ions into BH₄⁻ and BX₄⁻ becomes thermodynamically more favored with increasing electronegativity of the substituent X. Characterization of the new hydrido borate species is usually unambiguous, but Li[H₂BO(C₆H₄)₂] (10) shows an anomalous temperature dependent behavior in THF solution which can be attributed to an equilibrium involving Li(2H, 20), Li(2H, 30), and Li(30) structural units. This is supported by the x-ray structure of dimeric 10·THF and monomeric 10·THF·TMEDA. While 9·3THF is monomeric and contains doubly bridging H₂B groups, all other dihydrido diorganyl borates are dinuclear. The interaction between the alkali metal center and the boron bonded H atoms depends on number and size of the auxiliary ligands. Agostic Li...H-C interactions play a role if β-H atoms are present and when the alkali metal cation is not coordinatively saturated by the auxiliary ligand and the H(B) hydrogens. The most sym. and so far unique arrangement is found for [6a·2THF]₂ where all four H(B) hydrogens form Li...H...Li bridges. Also lithium bis(dithiocatecholato)borate, 17·2THF is dimeric. Its Li

centers are coordinated by four sulfur and two oxygen atoms. These atoms form a double heterocubane structure with two diametral edges missing.

IT 326500-96-3P
(preparation and crystal and mol. structure)
RN 326500-96-3 HCAPLUS
CN Lithium, [[1,1'-biphenyl]-2,2'-diyldihydroborato(1-)]tris(tetrahydrofuran)- (9CI) (CA INDEX NAME)



IT 13059-59-1, 9-Chloro-9-borafluorene
(reactant for preparation of alkali metal dihydridoborate complexes)
RN 13059-59-1 HCAPLUS
CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 29, 75
IT 326500-91-8P 326500-92-9P 326500-96-3P 326500-98-5P
326501-02-4P 326501-04-6P 326501-05-7P
(preparation and crystal and mol. structure)
IT 110-18-9, Tmeda 120-80-9, Catechol, reactions 142-29-0,
Cyclopentene 540-63-6, 1,2-Ethanedithiol 592-42-7,
1,5-Hexadiene 3030-47-5, Pmdta 5158-50-9, Bromodimethylborane
7580-67-8, Lithium hydride (LiH) 7693-26-7, Potassium hydride
(KH) 13059-59-1, 9-Chloro-9-borafluorene 13283-31-3,
Borane, reactions 16949-15-8, Lithium borohydride (LiBH4)
17534-15-5, 1,2-Benzenedithiol 19091-73-7 21205-91-4,
9-Borabicyclononane dimer 81175-90-8, Chlorodi(tert-butyl)borane
201858-00-6
(reactant for preparation of alkali metal dihydridoborate complexes)
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L12 ANSWER 16 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

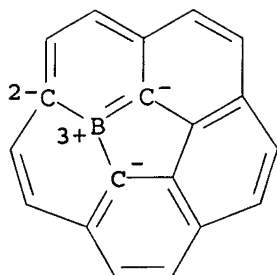
ACCESSION NUMBER: 2000:893718 HCAPLUS
DOCUMENT NUMBER: 134:295428
TITLE: The role of heteroatom substitution in the rigidity and curvature of buckybowls. A theoretical study
AUTHOR(S): Sastry, G. Narahari; Priyakumar, U. Deva
CORPORATE SOURCE: Department of Chemistry, Pondicherry University, Pondicherry, 605 014, India
SOURCE: Journal of the Chemical Society, Perkin Transactions 2 (2001), (1), 30-40
CODEN: JCSPGI; ISSN: 1472-779X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ab initio (Hartree Fock), hybrid d. functional (B3LYP), and semiempirical SCF (MNDO and AM1) calcns. on sumanene (I), trioxa-sumanene and trithia-sumanene show that the C3v-bowl structure is a min. in all cases, but show dramatic variations in bowl depths and inversion barriers. Calcns. on monosubstituted corannulenes C19XH10 (X = N+, B-, P+ and Si) at various levels predict that isoelectronic substituents possessing large atomic size increase the bowl-to-bowl inversion barrier at the hub position and decrease it at the rim position. Strain is a guiding factor, which accounts for the relative stability of positional isomers, curvature and bowl rigidity. The most stable positional isomer for a given substituent shows the min. bowl-to-bowl inversion barrier in all cases. Calcns. are performed on monosubstituted sumanenes derived by replacing skeletal C by isoelectronic atoms on I, C20XH12 for X = N+ and Si. The general strategy of substituting larger atoms at rim positions flattens the bowl, and at the hub position it makes the bowl deeper. The strategy seems to work well. HF/3-21G and B3LYP/6-31G* computations are in very good agreement with each other, both qual. and quant., and the central results are reproducible even at semiempirical levels. The performance of MNDO is consistently better than AM1 and becomes the method of choice when ab initio and DFT methods are not practical. Homodesmic equations, used to ascertain the thermodyn. stabilities of the monosubstitutions on corannulenes and sumanenes, show that substitution at appropriate sites imparts stability to the buckybowl framework. Linear correlation is obtained between the curvature, as estimated by the pyramidalization angle (Φ), and the inversion barrier. It is shown that bowl rigidity, curvature and the relative stabilities of positional isomers are controlled by the strain energy build up, which depends on the size of the substituent and the site of substitution.

IT 285571-27-9
(effect of heteroatom substitution on rigidity and curvature of buckybowls)

RN 285571-27-9 HCAPLUS

CN Borate(1-), 3,6-[1,4]pentadiene[1,5]diylphenanthrene-4,5-diyl-13-ylidene- (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)

Section cross-reference(s): 25

IT 5821-51-2, Corannulene 151253-59-7, Sumanene 251991-63-6
 260353-02-4 285571-27-9 285571-28-0 285571-29-1
 285571-30-4, 10b-Siladibenzo[ghi,mno]fluoranthene 285571-31-5
 285571-32-6 285571-33-7 285571-34-8, 2a-
 Siladibenzo[ghi,mno]fluoranthene 285571-35-9 285571-36-0
 285571-37-1 285571-38-2, Benzo[6,7]fluorantheno[1,10-bcd]silin
 334541-82-1 334541-83-2 334541-84-3 334541-85-4
 334541-86-5 334541-87-6 334541-88-7 334541-89-8
 (effect of heteroatom substitution on rigidity and curvature of
 buckybowls)

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L12 ANSWER 17 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:851558 HCAPLUS

DOCUMENT NUMBER: 134:163087

TITLE: New Fluorinated 9-Borafluorene Lewis Acids

AUTHOR(S): Chase, Preston A.; Piers, Warren E.; Patrick,
 Brian O.

CORPORATE SOURCE: Department of Chemistry, University of
 Calgary, Calgary, AB, T2N 1N4, Can.

SOURCE: Journal of the American Chemical Society
 (2000), 122(51), 12911-12912
 CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:163087

AB The synthesis of the fluorinated biphenyl-based borole derivs.
 (C12F8)B-R [R = CH3 (1a), C6F5 (1b), Br (1c)] and demonstrate
 their enhanced Lewis acidity relative to the more heavily
 fluorinated (C6F5)2B-R analogs is reported. Thus, lithiation of
 C12F8Br2 with BuLi followed by treatment with Me2SnCl2 in Et2O
 gave 80% C12F8SnMe2 which on treatment with BBr3 gave 77% C12F8BBR
 1c. Reaction of 1c with Cp2ZrMe2 gave 1a, whereas reaction of
 C12F8SnMe2 with Cl2BC6F5 gave 1b. 1a and 1b reacted with Cp2ZrMe2
 to give contact ion pairs. The crystal structure of 1b and
 contact ion pair of 1a with Cp2ZrMe2 is determined. The activation of
 metallocene catalysts by 1a and 1b for ethylene polymerization and MNDO
 calcs. for Lewis acidity of 1a and 1b and related derivs. is also
 reported.

IT 324766-71-4P
 (preparation and crystal structure of)

RN 324766-71-4 HCAPLUS

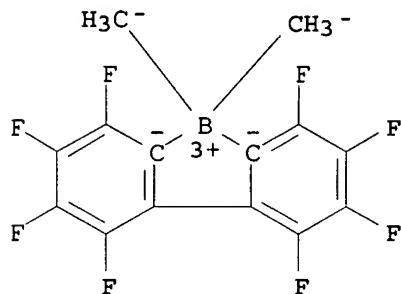
CN Zirconium(1+), bis(η^5 -2,4-cyclopentadien-1-yl)methyl-,
(T-4)-dimethyl(3,3',4,4',5,5',6,6'-octafluoro[1,1'-biphenyl]-2,2'-
diyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 324766-70-3

CMF C14 H6 B F8

CCI CCS

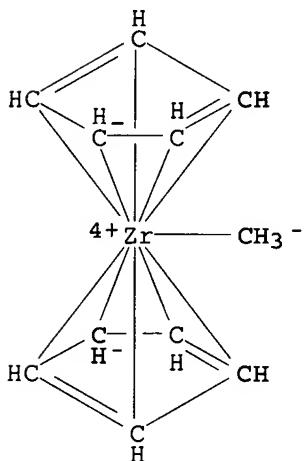


CM 2

CRN 94370-49-7

CMF C11 H13 Zr

CCI CCS

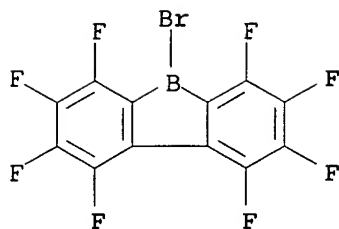


IT 324766-57-6P

(preparation and methylation of)

RN 324766-57-6 HCAPLUS

CN 5H-Dibenzoborole, 5-bromo-1,2,3,4,6,7,8,9-octafluoro- (9CI) (CA
INDEX NAME)



IT 324766-79-2P

(preparation of)

RN 324766-79-2 HCAPLUS

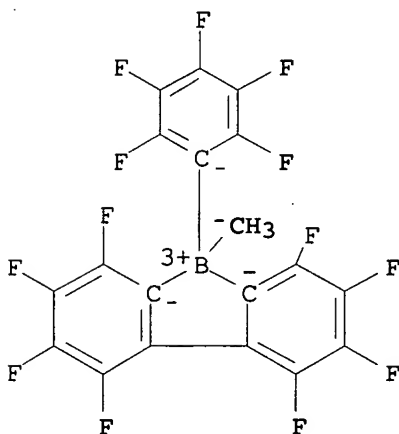
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-,
(T-4)-methyl(3,3',4,4',5,5',6,6'-octafluoro[1,1'-biphenyl]-2,2'-
diyl)(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 324766-78-1

CMF C19 H3 B F13

CCI CCS

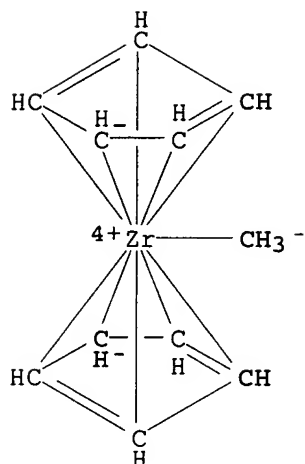


CM 2

CRN 94370-49-7

CMF C11 H13 Zr

CCI CCS

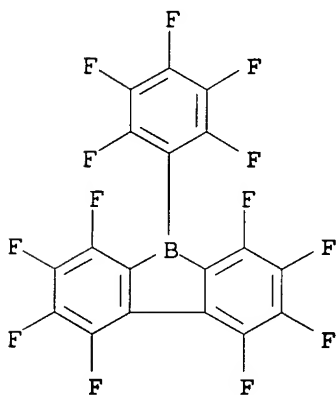


IT 324766-65-6P

(preparation, crystal structure, preparation of contact ion pair with dimethylzirconocene, MNDO calcn., and ethylene polymerization cocatalysis with)

RN 324766-65-6 HCAPLUS

CN 5H-Dibenzoborole, 1,2,3,4,6,7,8,9-octafluoro-5-(pentafluorophenyl)- (9CI) (CA INDEX NAME)

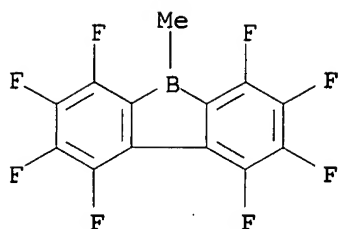


IT 324766-61-2P

(preparation, preparation of contact ion pair with dimethylzirconocene, MNDO calcn., and ethylene polymerization cocatalysis with)

RN 324766-61-2 HCAPLUS

CN 5H-Dibenzoborole, 1,2,3,4,6,7,8,9-octafluoro-5-methyl- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 35, 75

IT 324766-71-4P

(preparation and crystal structure of)

IT 324766-57-6P

(preparation and methylation of)

IT 9002-88-4P, Polyethylene 324766-79-2P

(preparation of)

IT 324766-65-6P

(preparation, crystal structure, preparation of contact ion pair with dimethylzirconocene, MNDO calcn., and ethylene polymerization cocatalysis with)

IT 324766-61-2P

(preparation, preparation of contact ion pair with dimethylzirconocene, MNDO calcn., and ethylene polymerization cocatalysis with)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 18 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:295981 HCAPLUS

DOCUMENT NUMBER: 133:120386

TITLE: Effect of substitution on the curvature and bowl-to-bowl inversion barrier of bucky-bowls. Study of mono-substituted corannulenes (C19XH10, X = B-, N+, P+ and Si)

AUTHOR(S): Sastry, G. Narahari; Prakash Rao, H. Surya; Priyakumar, U. Deva; Bednarek, Pawel

CORPORATE SOURCE: Dep. Chem., Pondicherry Univ., Pondicherry, 605014, India

SOURCE: Chemical Communications (Cambridge) (2000), (10), 843-844

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

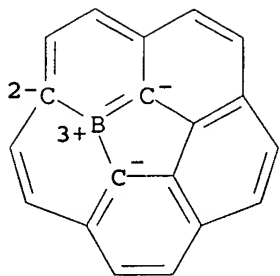
AB Ab initio MO and DFT calcns. predict that replacement of a single carbon by an isoelectronic species on the corannulene skeleton can effectively arrest the bowl shape or flatten it and the bowl rigidity, curvature and relative stabilities of the positional isomers are solely controlled by the size of the substituent and site of substitution.

IT 285571-27-9

(effect of substitution on curvature and bowl-to-bowl inversion barrier of bucky-bowls and study of mono-substituted bora-, aza-, phospho-, and sila-corannulenes)

RN 285571-27-9 HCAPLUS

CN Borate(1-), 3,6-[1,4]pentadiene[1,5]diylphenanthrene-4,5-diyl-13-ylidene- (9CI) (CA INDEX NAME)



CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 285571-27-9 285571-28-0 285571-29-1 285571-30-4,
 10b-Siladibenzo[ghi,mno]fluoranthene 285571-31-5 285571-32-6
 285571-33-7 285571-34-8, 2a-Siladibenzo[ghi,mno]fluoranthene
 285571-35-9 285571-36-0 285571-37-1 285571-38-2,
 Benzo[6,7]fluorantheno[1,10-bcd]silin
 (effect of substitution on curvature and bowl-to-bowl inversion
 barrier of bucky-bowls and study of mono-substituted bora-,
 aza-, phospho-, and sila-corannulenes)

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L12 ANSWER 19 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:566086 HCAPLUS

DOCUMENT NUMBER: 131:200269

TITLE: Metallocene catalysts for the polymerization
 of olefins

INVENTOR(S): Bohnen, Hans; Fritze, Cornelia; Kuber, Frank

PATENT ASSIGNEE(S): Targor GmbH, Germany

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9943717	A1	19990902	WO 1999-EP956	1999 0213
<--				
DE 19808253	A1	19990902	DE 1998-19808253	1998 0227
<--				
EP 1058694	A1	20001213	EP 1999-911664	1999 0213
<--				

EP 1058694 B1 20030409
 R: DE, ES, FR, GB, IT, NL
 JP 2002504596 T2 20020212 JP 2000-533466
 1999
 0213
 <--
 ES 2194449 T3 20031116 ES 1999-911664
 1999
 0213
 <--
 US 6391989 B1 20020521 US 2000-622417
 2000
 0816
 <--
 PRIORITY APPLN. INFO.: DE 1998-19808253 A
 1998
 0227
 <--
 WO 1999-EP956 W
 1999
 0213
 <--

OTHER SOURCE(S): MARPAT 131:200269

AB The title catalysts, which have the advantages of bulky ligands without the disadvantages of bulky aryl ligands, comprise complexes of Group IA, IIA, or IIIA metals with biphenyl derivs. of specified structure, metallocenes, and supports. Stirring 10 mmol 2,2'-dibromooctafluorobiphenyl (prepared by coupling 1,2-dibromotetrafluorobenzene with BuLi-TiCl₄) with 8 mL 2M BuLi in Et₂O at -78°, adding 5 mL 1M BCl₃, warming to room temperature, stripping solvent in vacuo, adding pentane and 0.79 g PhNMe₂.HCl, and stirring for 5 h gave N,N-dimethylanilinium bis(2,2'-octafluorobiphenyl)borate (I). Stirring 7.3 mg I, 5.9 mg dimethylsilylenebis(2-methyl-4-phenylindenyl)dimethylzirconium, and 1 g SiO₂ in PhMe and drying in vacuo gave a supported catalyst. Stirring 1.5 L liquid C₃H₆ with 3 mL 20% iso-Bu₃Al and the above catalyst at 60° for 1 h gave 214 g powdered polypropylene (37 kg/g metallocene-h).

IT 240419-12-9 240419-14-1

(metallocene catalysts for the polymerization of olefins)

RN 240419-12-9 HCAPLUS

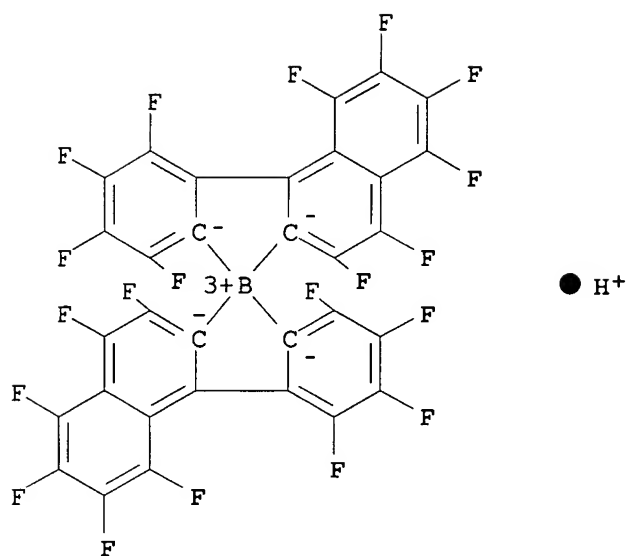
CN Borate(1-), bis[(3,4,5,6,7,8-hexafluoro-2,1-naphthalenediyl)(3,4,5,6-tetrafluoro-1,2-phenylene)]-, (T-4)-, hydrogen, compd. with N,N-dimethylbenzenamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 240419-11-8

CMF C32 B F20 . H

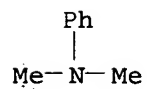
CCI CCS



CM 2

CRN 121-69-7

CMF C8 H11 N



RN 240419-14-1 HCAPLUS

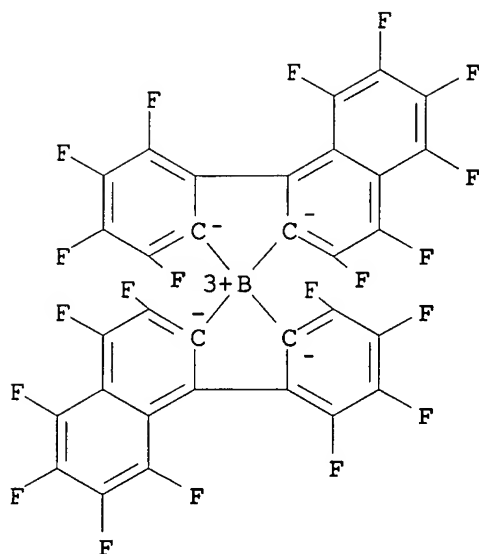
CN Methylum, triphenyl-, (T-4)-bis[(3,4,5,6,7,8-hexafluoro-2,1-naphthalenediyl) (3,4,5,6-tetrafluoro-1,2-phenylene)]borate(1-)
(9CI) (CA INDEX NAME)

CM 1

CRN 240419-13-0

CMF C32 B F20

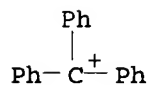
CCI CCS



CM 2

CRN 13948-08-8

CMF C19 H15



IT 238096-43-0P 238096-45-2P

(metallocene catalysts for the polymerization of olefins)

RN 238096-43-0 HCAPLUS

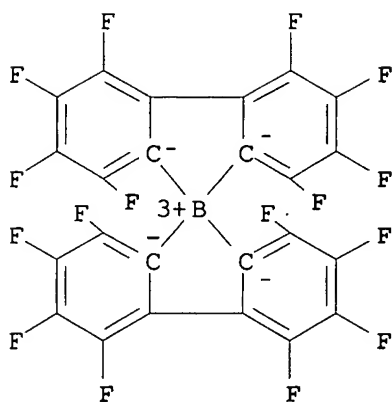
CN Borate(1-), bis(3,3',4,4',5,5',6,6'-octafluorobiphenyl)-2,2'-diyl-, (T-4)-, hydrogen, compd. with N,N-dimethylbenzenamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 238096-42-9

CMF C24 B F16 . H

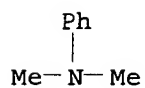
CCI CCS



CM 2

CRN 121-69-7

CMF C8 H11 N



RN 238096-45-2 HCAPLUS

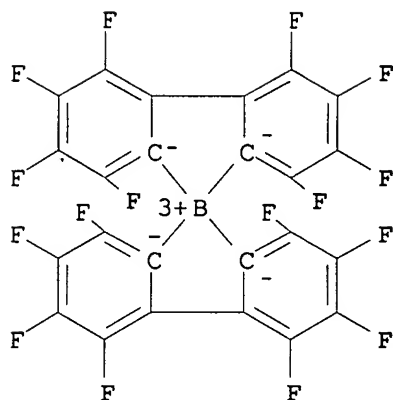
CN Methylium, triphenyl-, (T-4)-bis(3,3',4,4',5,5',6,6'-octafluoro[1,1'-biphenyl]-2,2'-diyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 238096-44-1

CMF C24 B F16

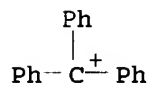
CCI CCS



CM 2

CRN 13948-08-8

CMF C19 H15



IC ICM C08F004-643

ICS C08F010-06

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

IT 1291-32-3 73364-10-0 119445-92-0 119821-97-5 135072-61-6

135571-35-6 135571-36-7 143278-90-4 143278-92-6

149342-08-5 152071-12-0 152881-64-6 152881-65-7

152881-66-8 152881-67-9 158238-79-0 158238-80-3

158515-16-3 161442-55-3 162426-41-7 162426-43-9

162857-08-1 163403-18-7 166601-14-5 167021-59-2

167254-77-5 168466-11-3 168749-19-7 168749-20-0

168749-22-2 168749-23-3 168749-24-4 168749-25-5

177991-18-3 187541-23-7 205745-71-7 205745-72-8

205745-73-9 207792-27-6 207792-28-7 213381-93-2

213381-94-3 213468-18-9 213922-27-1 238414-71-6

238414-72-7 238414-73-8 238414-74-9 238414-75-0

238414-76-1 238414-77-2 238414-81-8 238414-82-9

238414-83-0 238414-84-1 238414-87-4 238414-90-9

238414-92-1 238414-99-8 238415-03-7 238415-05-9

238415-07-1 238415-09-3 238415-11-7 238415-13-9

238415-15-1 238415-17-3 238415-18-4 238415-19-5

238415-20-8 238415-21-9 238415-23-1 238415-24-2

238432-64-9 238432-65-0 238432-66-1 238432-67-2

238432-68-3 238432-69-4 238432-70-7 238432-71-8

240419-12-9 240419-14-1 240419-17-4

240489-10-5

(metallocene catalysts for the polymerization of olefins)

IT 238096-43-0P 238096-45-2P 240419-08-3P

240419-10-7P

(metallocene catalysts for the polymerization of olefins)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE

FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L12 ANSWER 20 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1999:566055 HCAPLUS
 DOCUMENT NUMBER: 131:170472
 TITLE: Compounds having an ionic structure used as
 constituent of an olefin polymerization
 catalyst
 INVENTOR(S): Bohnen, Hans; Fritze, Cornelia; Kuber, Frank
 PATENT ASSIGNEE(S): Targor GmbH, Germany
 SOURCE: PCT Int. Appl., 22 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9943685	A1	19990902	WO 1999-EP957	1999 0213
<--				
W: BR, CN, JP, KR, US RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19808254	A1	19990902	DE 1998-19808254	1998 0227
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EP 1058685	A1	20001213	EP 1999-908893	1999 0213
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EP 1058685	B1	20030528		
R: DE, ES, FR, GB, IT, NL				
JP 2002504556	T2	20020212	JP 2000-533438	1999 0213
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ES 2201679	T3	20040316	ES 1999-908893	1999 0213
<--				
US 6437187	B1	20020820	US 2000-622418	2000 0816
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PRIORITY APPLN. INFO.:			DE 1998-19808254	A 1998 0227
<--				
			WO 1999-EP957	W 1999 0213
<--				

OTHER SOURCE(S): CASREACT 131:170472; MARPAT 131:170472
 AB The invention relates to chemical compds. having an ionic structure,

[M1Q1xQ2yQ3z]-A+ (M1 = group IIA, IIIA, IVA, VA element, x, y, z = 0-1, A = cation of group IA, IIA, IIIA element, carbenium, oxonium, phosphonium, sulfonium cation, Q = biphenyl ligand compds.), which in combination with an organometallic transition compound form a catalyst system which can advantageously be used to polymerize olefins. Thus, lithiation of 2,2'-dibromooctafluorobiphenyl with BuLi in Et₂O followed by sequential treatment with BCl₃ and N,N-dimethylanilinium chloride gave title compound, N,N-dimethylanilinium bis(2,2'-octafluorobiphenyl)borate.

IT 238096-43-0P 238096-45-2P

(preparation of compds. having ionic structure used as constituent of olefin polymerization catalyst)

RN 238096-43-0 HCAPLUS

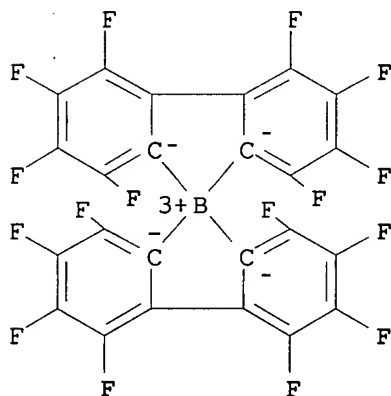
CN Borate(1-), bis(3,3',4,4',5,5',6,6'-octafluoro[1,1'-biphenyl]-2,2'-diyl)-, (T-4)-, hydrogen, compd. with N,N-dimethylbenzenamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 238096-42-9

CMF C24 B F16 . H

CCI CCS

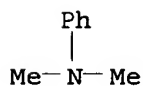


● H⁺

CM 2

CRN 121-69-7

CMF C8 H11 N



RN 238096-45-2 HCAPLUS

CN Methylum, triphenyl-, (T-4)-bis(3,3',4,4',5,5',6,6'-octafluoro[1,1'-biphenyl]-2,2'-diyl)borate(1-) (9CI) (CA INDEX

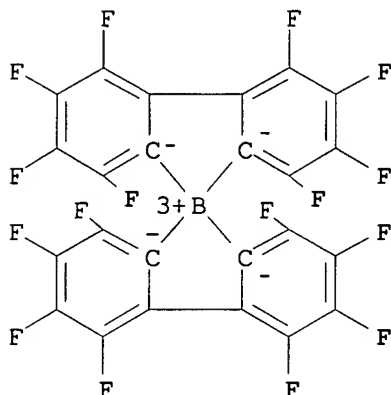
NAME)

CM 1

CRN 238096-44-1

CMF C24 B F16

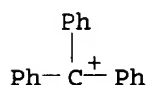
CCI CCS



CM 2

CRN 13948-08-8

CMF C19 H15



IC ICM C07F005-02

ICS C07F009-6568; C08F010-00

CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35

IT 238096-43-0P 238096-45-2P 238096-46-3P

238096-47-4P

(preparation of compds. having ionic structure used as constituent of olefin polymerization catalyst)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L12 ANSWER 21 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:597429 HCAPLUS

DOCUMENT NUMBER: 127:266902

TITLE: Co-carbonization of 9-chloroborfluorene and pitch; synthesis of B/C materials

AUTHOR(S): Hu, Raymond; Chung, T. C.

CORPORATE SOURCE: Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Carbon (1997), 35(8), 1101-1109

CODEN: CRBNAH; ISSN: 0008-6223

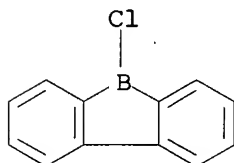
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper is a continuation of our research efforts in the development of boron containing carbon (B/C) materials. The chemical is based on the co-carbonization reaction between 9-chloroboratrafluorene precursor and FCC decant oil pitch. By adding small amts. of 9-chloroboratrafluorene, the yield of low temperature anisotropic carbon from the com. pitch was dramatically improved. This simple and effective method results in a broad range of B/C materials. In addition, the co-carbonization reaction provides direct evidence of boron-enhanced graphitization and the effect of boron content on crystal growth. In general, the graphitization temperature of pitch can be lowered by several hundred degrees by incorporating small amts. of boron precursor, and a large crystal size with low d-spacing, similar to Sp-1 graphite, is obtained at 2300°C.

IT 13059-59-1
(synthesis of boron-containing carbon materials by co-carbonization of 9-chloroboratrafluorene and pitch)

RN 13059-59-1 HCAPLUS

CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 57-8 (Ceramics)

IT 13059-59-1
(synthesis of boron-containing carbon materials by co-carbonization of 9-chloroboratrafluorene and pitch)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L12 ANSWER 22 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:467602 HCAPLUS

DOCUMENT NUMBER: 127:88071

TITLE: Borate photoinitiator from monoborane for photocurable material

INVENTOR(S): Cunningham, Allan Francis; Kunz, Martin; Kura, Hisatoshi

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Ger. Offen., 61 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19648256	A1	19970528	DE 1996-19648256	1996

				1121
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TW 467933	B	20011211	TW 1996-85113755	
				1996
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CH 691775	A	20011015	CH 1996-2824	
				1996
				1114
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AU 9671792	A1	19970529	AU 1996-71792	
				1996
				1115
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AU 712075	B2	19991028		
FR 2741624	A1	19970530	FR 1996-14200	
				1996
				1121
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FR 2741624	B1	19981204		
US 5932393	A	19990803	US 1996-755771	
				1996
				1121
			<--	
NL 1004599	A1	19970527	NL 1996-1004599	
				1996
				1122
			<--	
NL 1004599	C2	19980112		
GB 2307472	A1	19970528	GB 1996-24328	
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				1122
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GB 2307472	B2	19991117		
CN 1159450	A	19970917	CN 1996-121744	
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				1122
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BE 1010765	A5	19990105	BE 1996-980	
				1996
				1122
			<--	
ES 2126500	A1	19990316	ES 1996-2465	
				1996
				1122
			<--	
ES 2126500	B1	19991116		
AT 9602042	A	20000115	AT 1996-2042	
				1996
				1122
			<--	
AT 406777	B	20000925		
SG 49990	A1	20010116	SG 1996-11378	
				1996
				1122
			<--	
JP 09188710	A2	19970722	JP 1996-329222	
				1996
				1125
			<--	

BR 9605696	A	19980818	BR 1996-5696	1996 1125
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US 6045974	A	20000404	US 1999-247147	1999 0209
			<--	
PRIORITY APPLN. INFO.:			CH 1995-3344	A 1995 1124
			<--	
			US 1996-755771	A3 1996 1121
			<--	

OTHER SOURCE(S): MARPAT 127:88071

AB A photopolymerizable composition contains the borate photoinitiator [R1R2R3R4B]-.G+ or R2R3R4B-R1aE+ (R1, R2, R3 = Ph, aromatic hydrocarbyl with(out) heteroatom; R2 and R3 may form fused rings; R1a = divalent hydrocarbyl, Ph-C1-6-alkylene; G = pos. ion forming residue; E = R21R22R23P, R7R7aR8N, R6R6aS; R21, R22, R23 = C1-12-alkyl, C2-12-alkenyl, C3-12-cycloalkyl; R7, R7a, R8 = C1-12-alkyl, C3-12-cycloalkyl, Ph-C1-6-alkyl, Ph; R6, R6a = C1-12-alkyl, Ph-C1-6-alkyl, Ph) and a polymerizable ethylenic unsatd. compound. The photoinitiator may be used in coatings, printing inks, printing plates, dental materials, resist materials, stereolithog. materials, holog. recording materials, etc.

IT 191876-43-4P

(preparation of borate photoinitiator from borane)

RN 191876-43-4 HCAPLUS

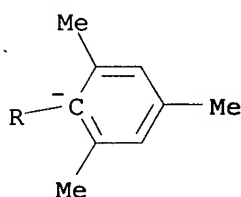
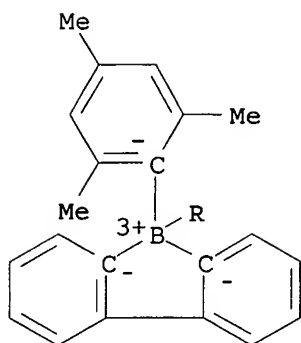
CN Methanaminium, N,N,N-trimethyl-, (T-4)-[1,1'-biphenyl]-2,2'-diylbis(2,4,6-trimethylphenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 191876-42-3

CMF C30 H30 B

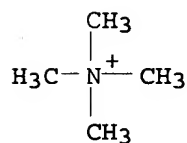
CCI CCS



CM 2

CRN 51-92-3

CMF C4 H12 N



IC ICM C08F002-46
 ICS C08F004-52; C07F005-02; C09J011-06; C08K005-55; C09B069-06;
 C09D004-00; C09D201-02; C09D005-46; C09D011-10; A61K006-00;
 G03F007-028

ICA C09D007-12; C09B011-28; C09B023-01; C09B057-00; C09B019-00;
 C09B017-00; C09B011-04; C09B021-00

CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and
 Other Reprographic Processes)
 Section cross-reference(s): 29, 35, 42

IT 191420-15-2P 191420-17-4P 191420-33-4P 191420-36-7P
 191420-89-0P 191420-93-6P 191420-95-8P 191420-97-0P
 191421-00-8P 191421-01-9P 191421-02-0P 191421-03-1P
 191421-04-2P 191875-98-6P 191875-99-7P 191876-00-3P
 191876-01-4P 191876-02-5P 191876-04-7P 191876-06-9P
 191876-07-0P 191876-08-1P 191876-10-5P 191876-12-7P
 191876-14-9P 191876-16-1P 191876-18-3P 191876-20-7P
 191876-22-9P 191876-24-1P 191876-26-3P 191876-28-5P
 191876-30-9P 191876-32-1P 191876-34-3P 191876-36-5P
 191876-38-7P 191876-39-8P 191876-40-1P 191876-41-2P
 191876-43-4P 191876-44-5P 191876-45-6P 191876-46-7P
 191876-47-8P 191876-48-9P 191876-49-0P 191876-50-3P

191876-51-4P 191876-52-5P 191876-53-6P
(preparation of borate photoinitiator from borane)

L12 ANSWER 23 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:270864 HCAPLUS
DOCUMENT NUMBER: 127:5118
TITLE: One-electron reductions of organodiborane(4)
compounds: singly reduced anions and
rearrangement reactions
AUTHOR(S): Grigsby, Warren J.; Power, Philip
CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA,
95616, USA
SOURCE: Chemistry--A European Journal (1997), 3(3),
368-375
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB One-electron redns. of the tetraaryldiborane(4) compound
Mes₂BBMes(Ph) (1) (Mes = 2,4,6-Me₃C₆H₂) with KC₈ to afford the
singly reduced radical anions [K(DME)₃][Mes₂BBMes(Ph)] (2) and
[K([18]crown-6)(THF)₂][Mes₂BBMes(Ph)] (3) are described. Both 2
and 3 were characterized by IR and EPR spectroscopy, and x-ray
diffraction studies of 3 showed it to be a solvent-separated ion pair.
Similarly, reduction of Mes(MeO)BB(OMe)Mes with lithium in di-Et ether
under controlled conditions furnished the radical anion
[Li(OEt)₂][Mes(MeO)BB(OMe)Mes] (4), which has a contact-ion-pair
structure in which lithium is solvated by oxygen atoms from ether
mols. and methoxy groups. The x-ray crystallog. studies of (3)
and (4) revealed shortened B-B bond lengths in both compds.,
consistent with the presence of partial (bond order 0.5) B-B π
bonds. Interestingly, the B-B distances in the singly reduced
species are very similar to those in the doubly reduced dianions
[R₂BBR₂]²⁻, which have found π -bond orders of unity. The
synthesis and characterization of 2,6-Mes₂C₆H₃(MeO)BB(OMe)₂ (5)
and 2,6-Mes₂C₆H₃(MeO)BB(OMe)Mes (6) are also reported. Reduction of 6
or 5 with lithium in di-Et ether solution did not lead to multiply
bonded B-B species, but to the isolation of the rearranged
products [(Et₂O)Li][1-mesityl-5,7-dimethyl-9-hydro-10-
{mesityl(methoxy)boryl}-10-boraphenanthrenyl] (7) and
[(Et₂O)₂Li][1-mesityl-5,7-dimethyl-9-methoxy-9'-
{methyl(methoxy)boryl}-9-borafluorenyl] (8), resp. Products 7 and
8 are derived from the intramol. insertion of the boron center
into C-H or C-C σ bonds. The crystal structure detns. of 5,
7, and 8 are also described.

IT 189942-72-1P
(preparation and crystal structure of)

RN 189942-72-1 HCAPLUS

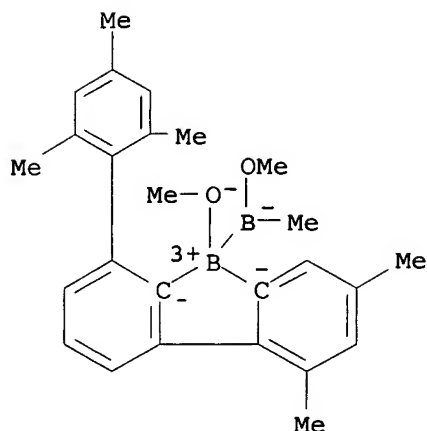
CN Lithium(1+), bis[1,1'-oxybis[ethane]]-, (T-4)-methoxy(methyl
methylborinato- κ B)(2'',4,4'',6,6''-pentamethyl[1,1':3',1''-
terphenyl]-2,2'-diyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 189942-71-0

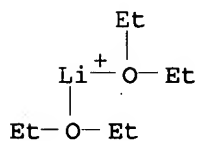
CMF C26 H31 B2 O2

CCI CCS



CM 2

CRN 78127-97-6
 CMF C8 H20 Li O2
 CCI CCS



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 72, 75

IT 189942-70-9P 189942-72-1P 190087-99-1P

(preparation and crystal structure of)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L12 ANSWER 24 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:679757 HCAPLUS

DOCUMENT NUMBER: 125:336863

TITLE: Synthesis and characterization of novel B/C
 materials prepared by 9-chloroboratrafluorene
 precursor

AUTHOR(S): Hu, Raymond; Chung, T. C.

CORPORATE SOURCE: Dep. of Materials Science and Engineering,
 Pennsylvania State Univ., University Park, PA,
 16802, USA

SOURCE: Carbon (1996), 34(10), 1181-1190

CODEN: CRBNAH; ISSN: 0008-6223

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper describes a novel boron-containing carbon (B/C) material
 which contains up to 7 mol% of boron atoms substitutionally
 incorporated in the graphite structure. The chemical involves the
 use of 9-chloroboratrafluorene precursor and the thermo-

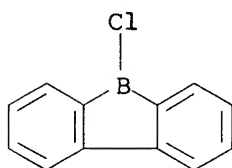
transformation reaction. 9-Chloroboratrafluorene was firstly oligomerized to mesophase boron-containing pitch (B-pitch) which is processable by solution and melt. The mesophase B-pitch was then pyrolyzed at various temps. ($\leq 2300^\circ$) to produce B/C material with high yield (.apprx.80%). During pyrolysis, boron is not only substitutionally incorporated in the graphitic structure but also enhances the graphitization reaction. An unusually large crystallite size and small d-spacing between interlayers of the B/C product was observed by x-ray diffraction.

IT 13059-59-1

(precursor; synthesis and characterization of B-containing graphite materials prepared by thermal decomposition of 9-chloroboratrafluorene precursor)

RN 13059-59-1 HCAPLUS

CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 57-8 (Ceramics)

Section cross-reference(s): 78

IT 13059-59-1

(precursor; synthesis and characterization of B-containing graphite materials prepared by thermal decomposition of 9-chloroboratrafluorene precursor)

L12 ANSWER 25 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:479406 HCAPLUS

DOCUMENT NUMBER: 125:221917

TITLE: Isolation and Reduction of Sterically Encumbered Arylboron Dihalides: Novel Boranediyl Insertion into C-C σ -Bonds

AUTHOR(S): Grigsby, Warren J.; Power, Philip P.

CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA

SOURCE: Journal of the American Chemical Society (1996), 118(34), 7981-7988

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:221917

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

AB The synthesis and subsequent reduction of the arylboron dihalides 2,6-Mes₂C₆H₃BX₂ (X = Cl (1); Br (2)) and 2,6-Trip₂C₆H₃BBr₂ (3) (Mes = 2,4,6-Me₃C₆H₂- and Trip = 2,4,6-i-Pr₃C₆H₂-) are described. Treatment of 2 with Li metal in Et₂O gave the novel Li

9-borafluorenyl compds. 4 (shown as I) and 5 (shown as II) in which the boranediyl intermediate has inserted into an o-Me-ring C-C σ -bond to form a borafluorenyl structure incorporating B in a delocalized five-membered ring. Boranediyl insertion into C-C σ -bonds, as distinct from boranediyl induced rearrangements involving C:C cleavage in delocalized aromatic substrates, is unknown. The main difference between the structures of these products is that 5 is dimerized as a consequence of the reduction in the number of solvating ethers. Reduction of 2 with KC8 gave the 9-borafluorenyl ate compds. 6 and 7 (shown as III; L = THF, C6H6). These products also result from C-C bond insertion by B as seen in 4 and 5. However, the delocalization is not observed owing to the addition of H (presumably from solvent) to the borons affording borate salts. Reduction of 3 with 3 equiv of KC8 furnishes the new diborate species 8 (shown as IV). This compound features as unique B-B bonded dianionic structure with a long (1.83(2) Å) B-B bond which arises from the association of two borate radical anion fragments that have a 9-borafluorenyl structure similar to those described above. 2-8 Were characterized by ^1H , ^{13}C , ^7Li , and ^{11}B NMR spectroscopy and by x-ray crystallog.

IT 180987-34-2P 180987-36-4P 180987-39-7P

181149-76-8P 181239-48-5P

(preparation and crystal structure of)

RN 180987-34-2 HCAPLUS

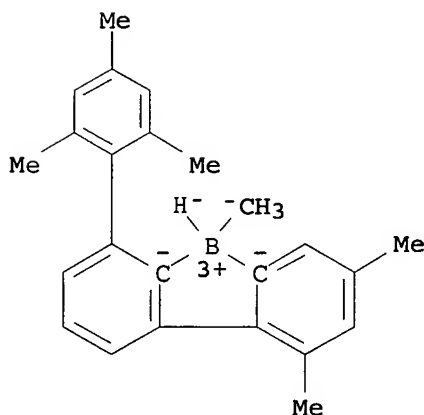
CN Potassium(1+), bis(tetrahydrofuran)-, (T-4)-hydromethyl[2'',4,4'',6,6''-pentamethyl[1,1':3',1''-terphenyl]-2,2'-diyl]borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 180987-33-1

CMF C24 H26 B

CCI CCS

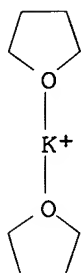


CM 2

CRN 73836-17-6

CMF C8 H16 K O2

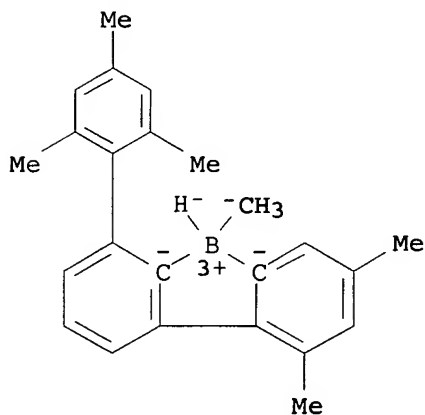
CCI CCS



RN 180987-36-4 HCAPLUS
 CN Borate(1-), hydromethyl[2'',4'',6,6''-pentamethyl[1,1':3',1''-terphenyl]-2,2'-diyl]-, (T-4)-, potassium, compd. with benzene (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 180987-35-3
 CMF C24 H26 B . K
 CCI CCS



● K⁺

CM 2

CRN 71-43-2
 CMF C6 H6



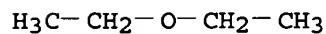
RN 180987-39-7 HCAPLUS

CN Potassium(1+), [1,1'-oxybis[ethane]]-, potassium dihydrobis[2'',4,4'',6,6''-pentakis(1-methylethyl)[1,1':3',1''-terphenyl]-2,2'-diyl]diborate(2-), compd. with 1,1'-oxybis[ethane] (2:2:2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 60-29-7

CMF C4 H10 O



CM 2

CRN 180987-38-6

CMF C66 H86 B2 . C4 H10 K O . K

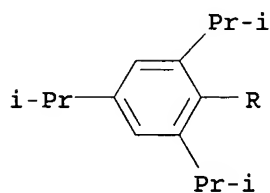
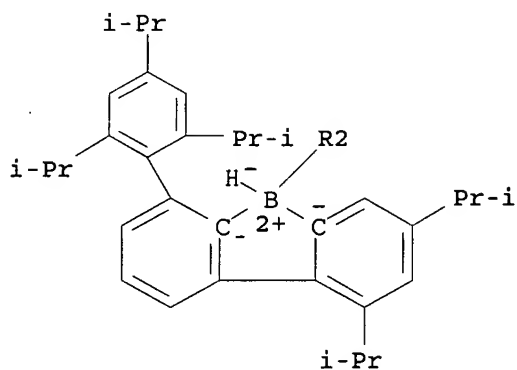
CM 3

CRN 180987-37-5

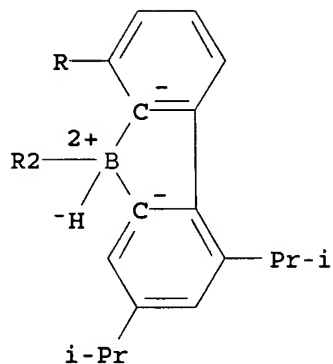
CMF C66 H86 B2

CCI CCS

PAGE 1-A



PAGE 2-A

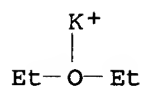


CM 4

CRN 120496-85-7

CMF C4 H10 K O

CCI CCS



RN 181149-76-8 HCAPLUS

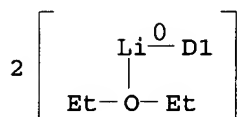
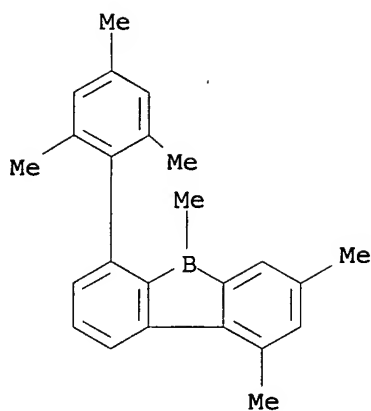
CN Lithium, [μ -[dihydro-1,3,5-trimethyl-6-(2,4,6-trimethylphenyl)-5H-dibenzoboroly]]bis[1,1'-oxybis[ethane]]di- (9CI) (CA INDEX NAME)

CM 1

CRN 181149-75-7

CMF C32 H43 B Li2 O2

CCI CCS, IDS

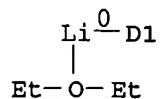
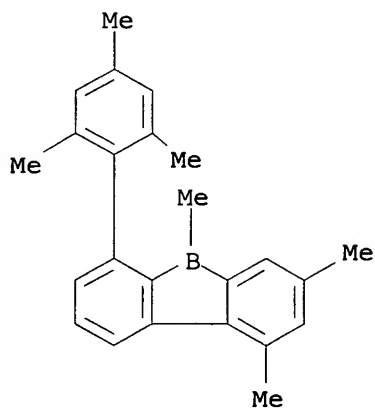


RN 181239-48-5 HCAPLUS
 CN Lithium, [μ -[dihydro-1,3,5-trimethyl-6-(2,4,6-trimethylphenyl)-5H-dibenzoborole-2-yl]] [1,1'-oxybis[ethane]]di- (9CI) (CA INDEX NAME)

CM 1

CRN 181239-47-4
 CMF C28 H33 B Li2 O
 CCI CCS, IDS

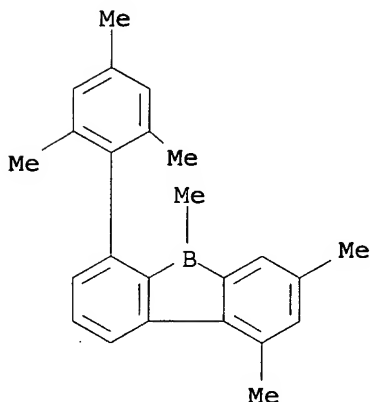
PAGE 1-A



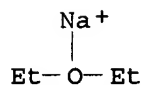
PAGE 2-A

D1-Li

IT 180987-41-1P
(preparation of)
RN 180987-41-1 HCAPLUS
CN Sodium(1+), [1,1'-oxybis[ethane]]-, salt with 1,3,5-trimethyl-6-(2,4,6-trimethylphenyl)-5H-dibenzoborole (1:1) (9CI) (CA INDEX NAME)
CM 1
CRN 180987-40-0
CMF C24 H25 B
CCI RIS



CM 2
CRN 23016-30-0
CMF C4 H10 Na O
CCI CCS



CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
IT 180987-34-2P 180987-36-4P 180987-39-7P
181149-76-8P 181239-48-5P
(preparation and crystal structure of)
IT 180987-41-1P
(preparation of)

L12 ANSWER 26 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:765704 HCAPLUS

USHA SHRESTHA EIC 1700 REM 4B28

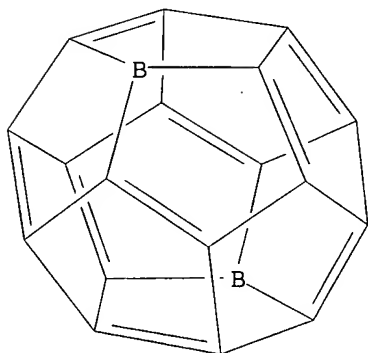
DOCUMENT NUMBER: 123:209188
 TITLE: Closed-shell electronic requirements for small fullerene cage structures
 AUTHOR(S): Fan, Man-Fai; Lin, Zhenyang; Yang, Shihe
 CORPORATE SOURCE: Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
 SOURCE: THEOCHEM (1995), 337(3), 231-40
 CODEN: THEODJ; ISSN: 0166-1280
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Hueckel model calcns. have been performed for small fullerene cages with 20-50 atoms. The closed-shell electronic structures for the small cages are emphasized. The relatively high stability of C₂₄, C₂₈, C₃₂, C₄₄ and C₅₀ clusters observed in the early laser vaporization expts. is explained. These clusters have pseudo closed-shell or half-filled electronic structures with a relatively large HOMO-LUMO gap. Based on the Heuckel results, a large number of other possible stable clusters is proposed formed by adding hydrogens, replacing carbons with other atoms which have an appropriate number of valence electrons, or encapsulating metal atoms capable of donating a given number of valence electrons.

IT 55518-39-3, 1,20-Dibora[5]fullerene-C₂₀-Ih
 (closed-shell electronic requirements for stability of)

RN 55518-39-3 HCAPLUS

CN 1,20-Dibora[5]fullerene-C₂₀-Ih (9CI) (CA INDEX NAME)

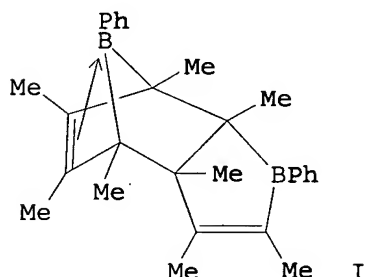


CC 65-3 (General Physical Chemistry)

IT 55518-39-3, 1,20-Dibora[5]fullerene-C₂₀-Ih 104375-45-3,
 [5]Fullerene-C₂₀-Ih 115383-19-2, Fullerene C₂₈ 115383-20-5,
 [5,6]Fullerene-C₃₂-D₃ 115383-21-6, [5,6]Fullerene-C₅₀-D_{5h}(6)
 135026-72-1, Fullerene C₃₀ 141175-42-0, [5,6]Fullerene-C₄₄-T_d
 142870-58-4, Fullerene C₂₄ 142870-59-5, Fullerene C₂₆
 144161-03-5, Fullerene C₃₆-D_{6h} 145646-79-3, Fullerene C₄₂-D₃
 146269-85-4, [5,6]Fullerene-C₄₄-D_{3h} 146269-86-5,
 [5,6]Fullerene-C₄₀-T_d 146269-87-6, Fullerene C₃₈-D_{3h}
 146401-64-1, [5,6]Fullerene-C₃₈-C_{3v} 153843-94-8,
 [5,6]Fullerene-C₃₄-C_{3v} 153843-95-9, [5,6]Fullerene-C₄₆-C₃
 153843-96-0, [5,6]Fullerene-C₄₈-D₃ 155475-37-9,
 [5,6]Fullerene-C₄₀-C_{3v} 156799-47-2, Fullerene-C₄₀ 168026-90-2
 (closed-shell electronic requirements for stability of)

L12 ANSWER 27 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:270663 HCAPLUS
 DOCUMENT NUMBER: 120:270663
 TITLE: Metallacycle Transfer from Zirconium to Main Group Elements: A Versatile Synthesis of Heterocycles
 AUTHOR(S): Fagan, Paul J.; Nugent, William A.; Calabrese, Joseph C.
 CORPORATE SOURCE: Central Research and Development Department, DuPont Company, Wilmington, DE, 19880-0328, USA
 SOURCE: Journal of the American Chemical Society (1994), 116(5), 1880-9
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 120:270663
 GI



AB The reaction of zirconium metallacycles is used to produce a variety of main group heterocycles including borole Diels-Alder dimers, galloles, indacyclopentadienes, siloles, germales, stannoles, phospholes, arsoles, stiboles, bismoles, thiophenes, selenophenes, dihydrothiophenes, dihydroselenophenes, tetrahydrothiophenes, tetrahydroselenophenes, stannacyclopentanes, phospholenes, and isothiazoles. An x-ray crystallog. study of the borole Diels-Alder dimer of 1-phenyl-2,3,4,5-tetramethylborole (I) is discussed and compared with the structure of 7-norbornenyl carbenium ions. The scope and potential for this metallacycle transfer reaction are delineated.

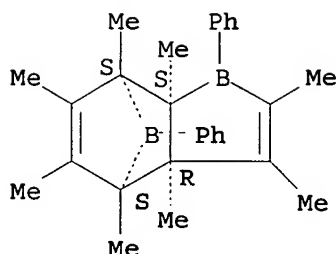
IT 113668-53-4P

(preparation and crystal and mol. structure of)

RN 113668-53-4 HCAPLUS

CN 4,7-Borylene-1H-1-benzoborole, 3a,4,7,7a-tetrahydro-
 2,3,3a,4,5,6,7,7a-octamethyl-1,8-diphenyl-, (3aR,4S,7S,7aS)-rel-
 (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT 113668-53-4P

(preparation and crystal and mol. structure of)

L12 ANSWER 28 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:270495 HCAPLUS

DOCUMENT NUMBER: 120:270495

TITLE: Rearrangements of organometallic compounds.

26. Bora-aromatic systems. 15. Skeletal rearrangements of arylborane complexes mediated by redox reactions: thermal and photochemical oxidation by metal ions

AUTHOR(S): Eisch, John J.; Shah, Jamshed H.; Boleslawski, Marek P.

CORPORATE SOURCE: Department of Chemistry, The State University of New York at Binghamton, Binghamton, NY, 13902-6000, USA

SOURCE: Journal of Organometallic Chemistry (1994), 464(1), 11-21

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:270495

AB A variety of metal salts are reduced by thermal and photochem. interaction with tetraarylborate salts and with neutral alkyl- and aryl-borane complexes. In the cases of Cu²⁺, Cu⁺, Ni²⁺, Co²⁺, Pd²⁺, Pt²⁺, Ag⁺, Zn²⁺, Hg²⁺, Sn²⁺, Pb²⁺ and Rh³⁺ salts, such photochem. redns. with NaBPh₄ led to the deposition of the free metal, while a number of binary mixts. of metal salts led to the codeposition of both metals, sometimes as true alloys, under such photoreductions. The arylborate reductants underwent oxidative coupling of the aryl groups to form biaryls in a strictly intra-ionic (for BAr₄⁻) or intramol. (Ar₃B) manner, resp. Individual studies of the photochem. of the tetraarylborate anion itself, of cuprous tetraphenylborate and of the triphenylborane-pyridine complex adduced evidence for a gamut of reactive intermediates capable of serving as the photoreductant for metal ions, such as triarylborane radical anions, diarylborate(I) anions or arylborenes, 7-borabicycloheptadiene anions or neutral complexes and finally arylborohydride anions or arylboron hydrides. The role of these intermediates both in the photoinduced skeletal rearrangements of arylboranes and in the concomitant reduction of metal ions is discussed in critical detail.

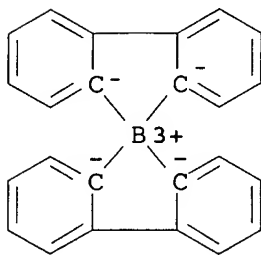
IT 54873-17-5P

(preparation and aryl coupling reaction of, with cupric bromide)

RN 54873-17-5 HCAPLUS

CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, sodium, (T-4)- (9CI)

(CA INDEX NAME)

● Na⁺

CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 78

IT 54873-17-5P

(preparation and aryl coupling reaction of, with cupric bromide)

L12 ANSWER 29 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:408897 HCAPLUS

DOCUMENT NUMBER: 119:8897

TITLE: Syntheses, structures, and spectroscopic studies of several new classes of compounds having boron-arsenic bonds

AUTHOR(S): Petrie, Mark A.; Olmstead, Marilyn M.; Hope, H.; Bartlett, Ruth A.; Power, Philip P.

CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA

SOURCE: Journal of the American Chemical Society (1993), 115(8), 3221-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 119:8897

AB Several new arsinoboranes, wherein boron and arsenic are three coordinate, have been prepared and characterized. They are analogous to B-N and B-P species in which p-p π -bonding, although inherently strong, is difficult to achieve because of the larger inversion barrier at arsenic. Nonetheless, very electropos. or bulky substituents at arsenic reduce this barrier sufficiently to observe substantial B-As π -interactions. The compound studied include [PhB(Cl)As(CMe₃)₂]₂ (1), PhB{As(CMe₃)₂]₂ (2), Cp*B(Cl)As(CMe₃)₂ (3), (C₂O₂H₃O)BAs(CMe₃)₂ (4), Mes₂BAsPhLi(THF)₃ (5), [Mes₂BAsPh][Li(TMEDA)₂] (6), and Mes₂BAs(Ph)SiMe₃ (7) (Cp* = pentamethylcyclopentadienyl, TMEDA = N,N'-tetramethylenediamine, Mes = 2,4,6-Me₃C₆H₂). The species 5 and 6 have been reported in a preliminary note. All compds. were characterized by X-ray crystallog. and ¹H NMR and ¹¹B NMR spectroscopy. In addition, 5 and 7 were characterized by variable-temperature ¹H NMR studies.

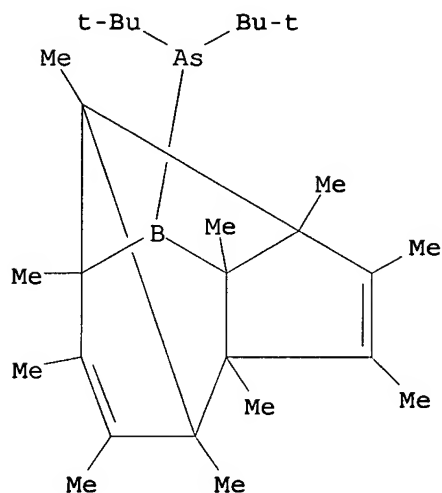
IT 147766-65-2P

(preparation and crystal and mol. structure of)

RN 147766-65-2 HCAPLUS

CN Arsine, bis(1,1-dimethylethyl) (5,5a,8,8a-tetrahydro-

2,3,4,5,5a,6,7,8,8a,9-decamethyl-2,5,8-methenocyclopenta[b]borepin-1(2H)-yl)-(9CI) (CA INDEX NAME)



CC 29-8 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT 147744-85-2P 147744-86-3P 147744-87-4P 147766-65-2P
(preparation and crystal and mol. structure of)

L12 ANSWER 30 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:7011 HCAPLUS

DOCUMENT NUMBER: 118:7011

TITLE: Diallenylboranes as starting molecules for boron heterocycles

AUTHOR(S): Enders, Markus; Pritzkow, Hans; Siebert, Walter

CORPORATE SOURCE: Anorg.-Chem. Inst., Univ. Heidelberg, Heidelberg, W-6900, Germany

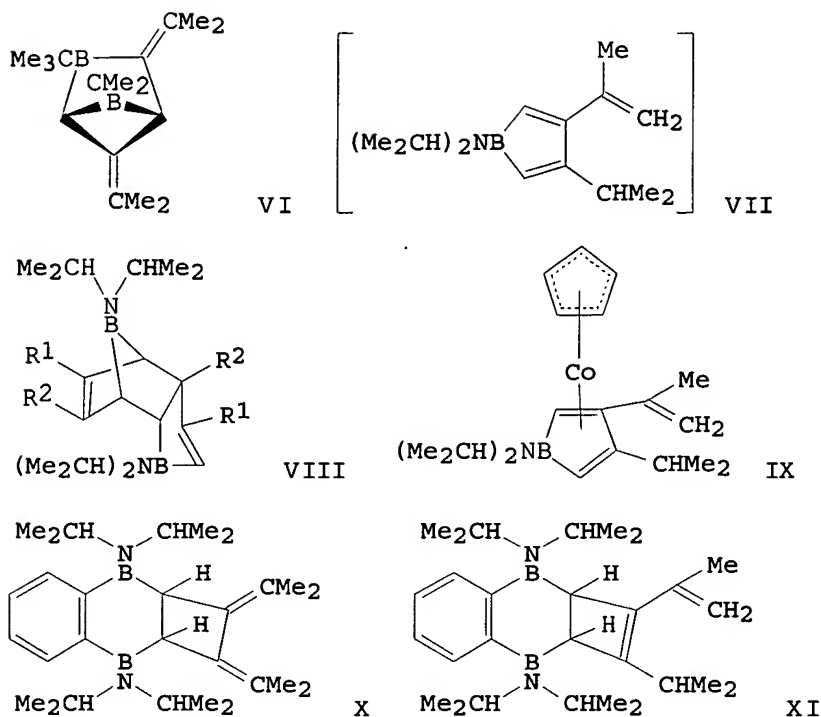
SOURCE: Chemische Berichte (1992), 125(9), 1981-5
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 118:7011

GI



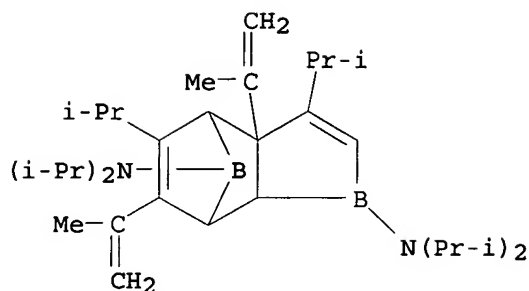
AB The reaction of allenyllithium with chloro(dialkylamino)boranes leads to the diallenylboranes $(\text{Me}_2\text{CH})_2\text{NB}(\text{CH}:\text{C}:\text{CMe}_2)_2$ (I), $\text{Me}_2\text{C}:\text{C}:\text{CHBRBRCH}:\text{C}:\text{CMe}_2$ [$\text{R} = \text{NMe}_2$ (II), CMe_3 (III)], and $\text{X}[\text{B}(\text{R})\text{CH}:\text{C}:\text{CMe}_2]_2$ [$\text{X} = \text{CH}_2$ (IV), $\text{R} = \text{NMe}_2$, $\text{N}(\text{CHMe}_2)_2$; $\text{X} = \text{o-C}_6\text{H}_4$, $\text{R} = \text{N}(\text{CHMe}_2)_2$ (V)] in 58-80% yields. Attempts to obtain III resulted in the formation of the unusual bicyclo compound VI. Heating I in toluene gives the intermediate borole derivative VII, which dimerizes to the Diels-Alder product VIII. Reaction of I with $(\text{C}_5\text{H}_5)\text{Co}(\text{C}_2\text{H}_4)_2$ leads to the cobalt-borole complex IX. No 1,5-H shift occurs on heating II and IV, resp. Heating V in mesitylene yields the diboratricycle X, which undergoes a photochem. 1,5-H shift to XI. Single crystal x-ray structure detns. of X, XI, and the complex IX confirm their constitutions.

IT 142363-08-4P

(preparation and spectra of)

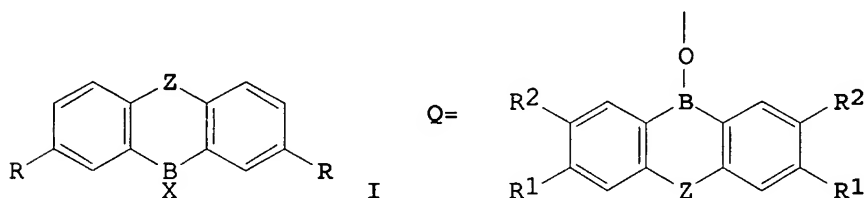
RN 142363-08-4 HCAPLUS

CN 4,7-Borylene-1H-1-benzoborole-1,8-diamine, 3a,4,7,7a-tetrahydro-3a,6-bis(1-methylethenyl)-N,N,N',N',3,5-hexakis(1-methylethyl)-, (3a α ,4 α ,7 α ,7a α) - (9CI) (CA INDEX NAME)

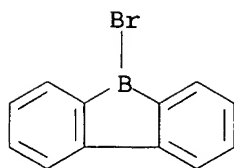


CC 29-4 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 IT 142363-05-1P 142363-06-2P 142363-08-4P 142363-11-9P
 (preparation and spectra of)

L12 ANSWER 31 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1991:408860 HCAPLUS
 DOCUMENT NUMBER: 115:8860
 TITLE: Electronic spectral study of conjugation in
 phenheteraborins
 AUTHOR(S): Kuznetsov, V. A.; Gamzatov, A. Z.; Barabonin,
 S. Yu.; Reikhsfel'd, V. O.; Nesterova, S. V.
 CORPORATE SOURCE: Astrakhan. Tekh. Inst. Rybn. Prom. Khoz.,
 Astrakhan, USSR
 SOURCE: Zhurnal Obshchei Khimii (1990), 60(11),
 2505-11
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB UV spectra of phenheteraborins (I; R = H, Me, Br; Z = O, NMe, Si,
 null; X = Ph, OCH2CH2NH2, OH, Br, 2Ph, Q; R1 = H, Me, Br; R2 = H,
 Br) were examined. A linear correlation exists between the
 frequencies of long-wave maximum in electron-transfer bands from HOMO
 to LUMO (ν_0) and frequencies of charge transfer (ν_{CT}). An
 aromatic π -electron system is confirmed, with n - π -p-conjugation
 in the heterocycle. The degree of aromaticity in I is similar to
 that in naphthalene and more condensed systems.
 IT 97322-60-6
 (UV spectrum of, aromaticity and conjugation in relation to)
 RN 97322-60-6 HCAPLUS
 CN 5H-Dibenzoborole, 5-bromo- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 18870-55-8 19014-28-9 95072-98-3 95925-64-7 95926-22-0
 97322-60-6 110156-13-3 112261-35-5 118450-94-5
 118450-96-7 134245-09-3 134266-42-5

(UV spectrum of, aromaticity and conjugation in relation to)

L12 ANSWER 32 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:122465 HCAPLUS

DOCUMENT NUMBER: 114:122465

TITLE: Derivatives of borole. XVII.
 [η^5 -[1-(Diisopropylamino)borole]]metal
 complexes: syntheses, protonation, internal
 rotation

AUTHOR(S): Herberich, Gerhard E.; Negele, Michael; Ohst,
 Holger

CORPORATE SOURCE: Inst. Anorg. Chem., Tech. Hochsch. Aachen,
 Aachen, D-5100, Germany

SOURCE: Chemische Berichte (1991), 124(1), 25-9
 CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 114:122465

GI For diagram(s), see printed CA Issue.

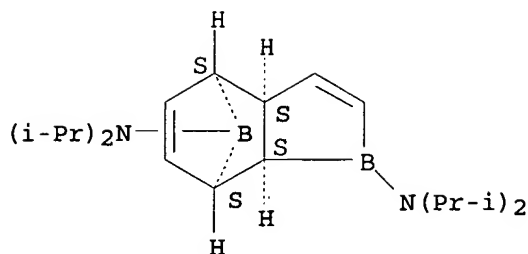
AB New complexes $M(\text{CO})_4\text{L}$ ($M = \text{Cr}, \text{W}$) and $\text{cis-}M(\text{CO})_2\text{L}_2$ [$M = \text{Mo}, \text{W}$ (not isolated)], and $(\text{COD})\text{NiL}$ ($\text{COD} = 1,5\text{-cyclooctadiene}$) were prepared from the Diels-Alder dimer L_2 (I), where L is 1-(diisopropylamino)borole, $\text{C}_4\text{H}_4\text{BN}(\text{CHMe}_2)_2$. Complexes of L can be protonated at the nitrogen atom to give stable salts such as $[\text{Cr}(\text{CO})_4(\text{LH})]\text{BF}_4$, $[\text{Fe}(\text{CO})_3(\text{LH})]\text{BF}_4$, $[(\text{C}_6\text{Me}_6)\text{Ru}(\text{LH})]\text{BF}_4$, and $[\text{CpCo}(\text{LH})]\text{BF}_4$ ($\text{Cp} = \eta^5\text{-cyclopentadienyl}$); B-N dissociation is not observed. Barriers to internal rotation were determined by variable temperature NMR spectroscopy for $\text{Cr}(\text{CO})_4\text{L}$, $(\text{COD})\text{NiL}$, and NiL_2 . Three processes were identified: rotation of the $\text{N}(\text{CHMe}_2)_2$ group around the B-N bond, gear-mesh rotation of the iso-Pr groups around the C-N bonds, and rotation of L with respect to the counter ligands.

IT 99610-64-7
 (reaction of, with metal carbonyl complexes)

RN 99610-64-7 HCAPLUS

CN 4,7-Borylene-1H-1-benzoborole-1,8-diamine, 3a,4,7,7a-tetrahydro-
 N,N,N',N'-tetrakis(1-methylethyl)-, (3a α ,4 α ,7 α ,7
 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 99610-64-7

(reaction of, with metal carbonyl complexes)

L12 ANSWER 33 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:53201 HCAPLUS

DOCUMENT NUMBER: 114:53201

TITLE: Structure of 2,10-bis(diisopropylamino)-1,5-dihydro-1,5-epiborano-2H-benzo[c]borepine

AUTHOR(S): Noltemeyer, Mathias; Pauer, Frank; Bromm, Dietmar; Meller, Anton

CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Goettingen, Goettingen, D-3400, Germany

SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1990), C46(10), 1981-2

CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE: Journal

LANGUAGE: English

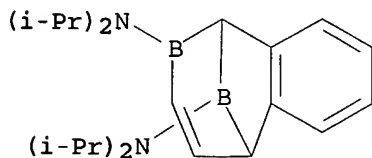
AB The title compound is monoclinic, space group C2/c, with a 10.701(9), b 17.789(9), c 24.143(12) Å, and $\beta = 90.84(3)^\circ$; d. (calculated) = 1.01 for Z = 8. Final R = 0.078 for 1450 reflections. Atomic coordinates are given. The compound was obtd. by borylation of naphthalene in such a way that one Bn[CH(CH3)2]2 unit has been added across one of the benzo rings, while the other has been inserted into the ring skeleton.

IT 131426-73-8

(crystal structure of)

RN 131426-73-8 HCAPLUS

CN 1,5-Borylene-2H-2-benzoborepin-2,10-diamine, 1,5-dihydro-N,N,N',N'-tetrakis(1-methylethyl)- (9CI) (CA INDEX NAME)



CC 75-8 (Crystallography and Liquid Crystals)

Section cross-reference(s): 29

IT 131426-73-8

(crystal structure of)

L12 ANSWER 34 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:552525 HCAPLUS
 DOCUMENT NUMBER: 113:152525
 TITLE: Boron-nitrogen compounds. 125. Pyrazole
 complexes of three-coordinated boranes
 AUTHOR(S): Komorowski, L.; Maringgele, W.; Meller, A.;
 Niedenzu, Kurt; Serwatowski, J.
 CORPORATE SOURCE: Dep. Chem., Univ. Kentucky, Lexington, KY,
 40506, USA
 SOURCE: Inorganic Chemistry (1990), 29(19), 3845-9
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 113:152525

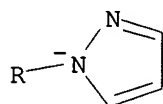
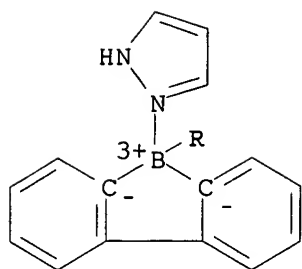
AB Both BF₃ and BEt₃ form 1:1 M complexes with pyrazole (Hpz) and C-substituted derivs. thereof. Provided the pyrazole is a relatively strong base, the BF₃ complexes slowly decompose on prolonged standing at room temperature with the elimination of HF to form the corresponding dimeric 1-pyrazolylboranes = pyrazaboles, e.g., F₂B(μ-pz)₂BF₂. Deprotonation of Hpz·BEt₃ with NaH yields the ion [Et₃B(pz)]⁻ and the salt K[Et₂B(pz)₂] is obtained on heating of an equimolar mixture of Hpz·BEt₃ and Kpz in Hpz. K[R₂B(pz)₂] are also obtained by the reaction of Me₂NBR₂, with Kpz and Hpz; they were converted to the representative Pd complexes Pd[(μ-pz)₂BEt₂]₂ and R₂B(μ-pz)₂Pd(π-CH₂CHCH₂) (R = Et, Pr, Ph), resp. Interaction of Me₂NBR₂ with 1 molar equivalent of Hpz gives 1:1 complexes Me₂HN·BR₂(pz), which can react with an addnl. molar equivalent of Hpz at elevated temps. to form Hpz·BR₂(pz), or form mixts. of the desired compound with the pyrazabole relative R₂B(μ-pz)[μ-NMe₂]BR₂. Steric factors may prevent the intermediate formation of the 1:1 complexes to lead directly to Hpz·BR₂(pz). The complexes Hpz·BR₂(pz) can be thermolyzed to yield the pyrazaboles R₂B(μ-pz)₂BR₂. However, whereas the reaction of [Me₂NBF₂]₂ with Hpz ultimately yields the pyrazabole F₂B(μ-pz)₂BF₂, the reaction of the cited aminoborane with Hpz and Kpz causes redistribution of fluorine and K[F₃B(pz)] is obtained as the only product containing B-F bonds. The complex (pz)₂BEt(H₂NMe) is formed on reaction of the borazine (EtBNMe₂)₃ with a large excess of Hpz, and H(pz)₃B(NHMe) is obtained in analogous fashion originating from the borazine Me₂NBNMe₃. The reaction of Me₂NNH₂B with excess Hpz yields the complex Me₂NNH₂·B(pz)₃.

IT 129391-30-6P

(preparation and thermolysis of)

RN 129391-30-6 HCAPLUS

CN Boron, [1,1'-biphenyl]-2,2'-diyl(1H-pyrazolato-N1)(1H-pyrazole-N2)-
 , (T-4)- (9CI) (CA INDEX NAME)

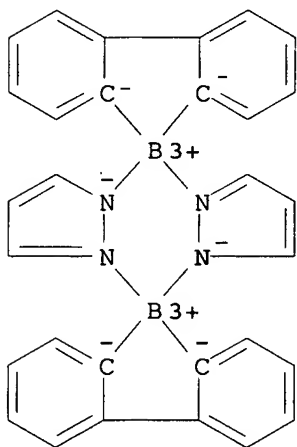


IT 129391-31-7P

(preparation of)

RN 129391-31-7 HCAPLUS

CN Boron, bis([1,1'-biphenyl]-2,2'-diyl)bis[μ-(1H-pyrazolato-N1:N2)]di- (9CI) (CA INDEX NAME)

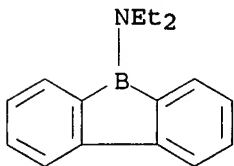


IT 97322-63-9

(reaction of, with pyrazole)

RN 97322-63-9 HCAPLUS

CN 5H-Dibenzoborol-5-amine, N,N-diethyl- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

IT 129391-30-6P

(preparation and thermolysis of)

IT 23218-84-0P 105336-02-5P 109744-75-4P 129391-16-8P
 129391-17-9P 129391-18-0P 129391-19-1P 129391-21-5P
 129391-22-6P 129391-23-7P 129391-24-8P 129391-26-0P
 129391-27-1P 129391-28-2P 129391-29-3P 129391-31-7P
 129391-32-8P 129391-33-9P 129391-34-0P 129391-35-1P
 129391-36-2P 129421-13-2P 129421-14-3P

(preparation of)

IT 715-62-8 6982-55-4 7397-47-9 16912-59-7 97322-63-9
 124927-05-5

(reaction of, with pyrazole)

L12 ANSWER 35 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:542214 HCAPLUS

DOCUMENT NUMBER: 113:142214

TITLE: Negatively charged electrophotographic toner

INVENTOR(S): Hsieh, Bing R.; Gruber, Robert J.; Haack, John L.

PATENT ASSIGNEE(S): Xerox Corp., USA

SOURCE: U.S., 10 pp.
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4898802	A	19900206	US 1989-354181	1989 0522
PRIORITY APPLN. INFO.:				1989 0522

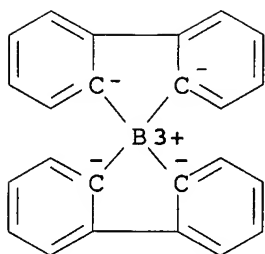
OTHER SOURCE(S): MARPAT 113:142214

AB A neg. charged electrophotog. toner comprises a resin, a pigment, and a charge-enhancing agent selected from the salts of 5,5'-spirobis(5H-dibenzoborole), 2,2',8,8'-tetramethoxy-5,5'-spirobi(5H-dibenzoborole), 3,3',7,7'-tetra-tert-butyl-5,5'-spirobi(5H-dibenzoborole), 2,2',8,8'-tetrafluoro-5,5'-spirobi(5H-dibenzoborole), and 2,2',3,3',7,7',8,8'-octamethoxy-5,5'-spirobi(5H-dibenzoborole). The electrophotog. toner containing the charge-enhancing agent shows triboelec. charging characteristics which are insensitive to humidity and is suited for a variety of electrophotog. imaging and printing processes including color xerog.

IT 108479-75-0 129433-65-4
 (charge-enhancing agent, for electrophotog. toners)

RN 108479-75-0 HCAPLUS

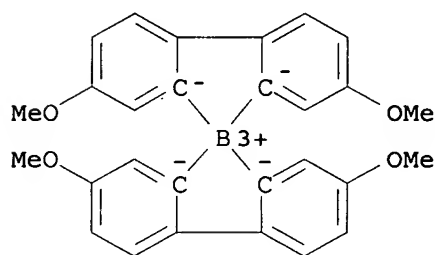
CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, lithium, (T-4)- (9CI)
 (CA INDEX NAME)



● Li⁺

RN 129433-65-4 HCAPLUS

CN Borate(1-), bis(4,4'-dimethoxy[1,1'-biphenyl]-2,2'-diyl)-, lithium, (T-4)- (9CI) (CA INDEX NAME)



● Li⁺

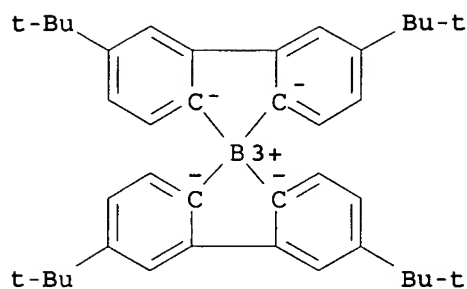
IT 128239-41-8D, salts 128239-42-9D, salts

128239-43-0D, salts

(charge-enhancing agents, for electrophotog. toners)

RN 128239-41-8 HCAPLUS

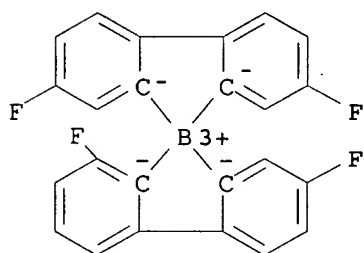
CN Borate(1-), bis[5,5'-bis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl]-, lithium, (T-4)- (9CI) (CA INDEX NAME)



● Li⁺

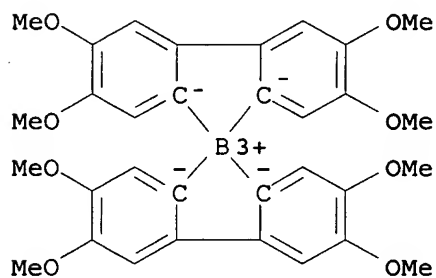
RN 128239-42-9 HCAPLUS

CN Borate(1-), bis(4,4'-difluoro[1,1'-biphenyl]-2,2'-diyl)-, (T-4)-
(9CI) (CA INDEX NAME)



RN 128239-43-0 HCAPLUS

CN Borate(1-), bis(4,4',5,5'-tetramethoxy[1,1'-biphenyl]-2,2'-diyl)-,
(T-4)- (9CI) (CA INDEX NAME)



IC ICM G03G009-08

INCL 430110000

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and
Other Reprographic Processes)

IT 108479-75-0 129433-65-4

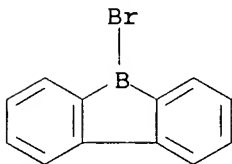
(charge-enhancing agent, for electrophotog. toners)

IT 128239-41-8D, salts 128239-42-9D, salts

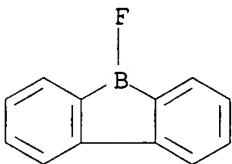
128239-43-0D, salts

(charge-enhancing agents, for electrophotog. toners)

L12 ANSWER 36 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:135284 HCAPLUS
DOCUMENT NUMBER: 110:135284
TITLE: A general, simple, and efficient synthesis of
fluoroorganoboranes
AUTHOR(S): Bir, Gerd; Schacht, Wolfgang; Kaufmann, Dieter
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg,
D-2000/13, Fed. Rep. Ger.
SOURCE: Journal of Organometallic Chemistry (1988),
340(3), 267-71
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 110:135284
AB The fluorination of a number of alkyl- and arylchloro- and
bromoboranes succeeds upon transhalogenation with lithium or
potassium fluoride under mild reaction conditions in good yields.
Thus, fluorination of 2-methylphenylboron dichloride with LiF in
Et2O gave 67% 2-MeC6H4BF2, whereas fluorination of
5-bromo-5H-dibenzoborole with KF in MeCN gave 73%
5-fluoro-5H-dibenzoborate.
IT 97322-60-6
(halogen exchange reaction of, with potassium fluoride)
RN 97322-60-6 HCAPLUS
CN 5H-Dibenzoborole, 5-bromo- (9CI) (CA INDEX NAME)



IT 119615-28-0P
(preparation of)
RN 119615-28-0 HCAPLUS
CN 5H-Dibenzoborole, 5-fluoro- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)
IT 97322-60-6 112150-12-6 112160-25-5
(halogen exchange reaction of, with potassium fluoride)
IT 86880-77-5P 112150-02-4P 119615-25-7P 119615-26-8P
119615-27-9P 119615-28-0P 119662-07-6P
(preparation of)

L12 ANSWER 37 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:186801 HCAPLUS
DOCUMENT NUMBER: 108:186801

TITLE: Synthesis of boroles and their use in low-temperature Diels-Alder reactions with unactivated alkenes

AUTHOR(S): Fagan, Paul J.; Burns, Elizabeth G.; Calabrese, Joseph C.

CORPORATE SOURCE: Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA

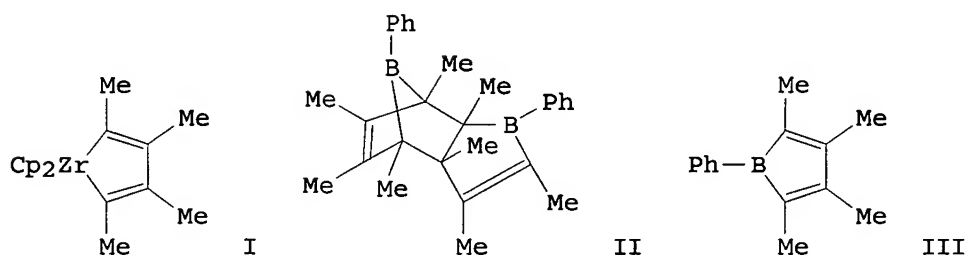
SOURCE: Journal of the American Chemical Society (1988), 110(9), 2979-81
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:186801

GI



AB Reaction of Zr metallacycle I with 1 equiv PhBCl_2 gave Cp_2ZrCl_2 ($\text{Cp} = \eta^5\text{-C}_5\text{H}_5$) and borole dimer II via the Diels-Alder dimerization of the intermediate 1-phenyl-2,3,4,5-tetramethylborole III. X-ray crystallog. shows that II has stereochem. resulting from endo addition of one borole ring upon the double bond of another, and that there is a non-classical interaction of the electron deficient bridgehead phenylboron group with the adjacent double bond indicative of sym. two electron-three center bonding. By a retro Diels-Alder reaction upon mild heating, II regenerates III in situ, which reacts with unactivated alkyne and alkenes, e.g., 2-butyne, ethylene, styrene, allyl chloride, cyclohexene, methylenecyclohexane, allene, 1,3-butadiene, and 1,3-cyclohexadiene, to give the corresponding Diels-Alder adducts in 63-94% yields.

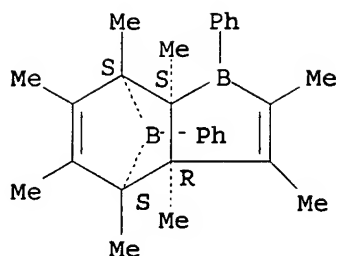
IT 113668-53-4P

(preparation and retro Diels-Alder reaction of, in presence of alkenes and alkynes)

RN 113668-53-4 HCAPLUS

CN 4,7-Borylene-1H-1-benzoborole, 3a,4,7,7a-tetrahydro-2,3,3a,4,5,6,7,7a-octamethyl-1,8-diphenyl-, (3aR,4S,7S,7aS)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.



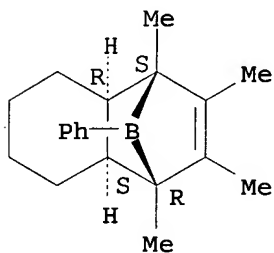
IT 113668-58-9P 113668-62-5P

(preparation of)

RN 113668-58-9 HCAPLUS

CN 1,4-Borylenenaphthalene, 1,4,4a,5,6,7,8,8a-octahydro-1,2,3,4-tetramethyl-9-phenyl-, (1 α ,4 α ,4a α ,8a α)-(9CI) (CA INDEX NAME)

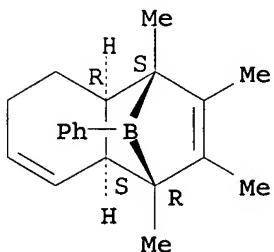
Relative stereochemistry.



RN 113668-62-5 HCAPLUS

CN 1,4-Borylenenaphthalene, 1,4,4a,5,6,8a-hexahydro-1,2,3,4-tetramethyl-9-phenyl-, (1 α ,4 α ,4a α ,8a α)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 29-4 (Organometallic and Organometalloidal Compounds)

IT 113668-53-4P

(preparation and retro Diels-Alder reaction of, in presence of alkenes and alkynes)

IT 113668-55-6P 113668-56-7P 113668-57-8P 113668-58-9P

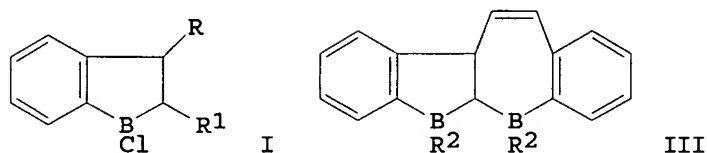
113668-59-0P 113668-60-3P 113668-61-4P 113668-62-5P

113668-63-6P

(preparation of)

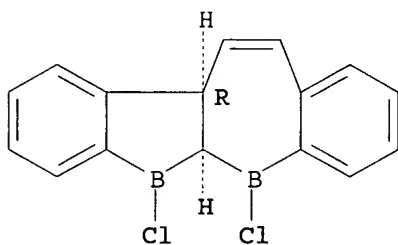
L12 ANSWER 38 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:477869 HCAPLUS
 DOCUMENT NUMBER: 107:77869
 TITLE: First synthesis of a benzoborole
 AUTHOR(S): Schacht, Wolfgang; Kaufmann, Dieter
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg,
 D-2000/13, Fed. Rep. Ger.
 SOURCE: Angewandte Chemie (1987), 99(7), 682-3
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 107:77869
 GI



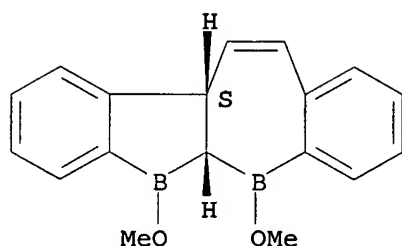
AB Flash vacuum pyrolysis of 2-EtC₆H₄BCl₂ at 900° gave the 1st example of title compound I (R₁ = bond) (II), which dimerizes to give 56% diboradibenzoazulene III (R₂ = Cl). The photoelectron spectrum of I (R = R₁ = H) at 925° also showed the presence of II. II was further confirmed by trapping expts. with MeC.tplbond.CMe, DCl, and MeOD to give 10% 1-chloro-2,3-dimethyl-1-benzoborepin, 50% E- and Z-2-DCH:CHC₆H₄BCl₂ (1:1 mixture), 35% Z-2-DCH:CHC₆H₄B(OMe)₂, and 15% III (R₂ = OMe).
 IT 108946-99-2P 108947-04-2P
 (preparation of)
 RN 108946-99-2 HCAPLUS
 CN [1]Benzoborolo[2,3-b][1]benzoborepin, 5,6-dichloro-5,5a,6,10b-tetrahydro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 108947-04-2 HCAPLUS
 CN [1]Benzoborolo[2,3-b][1]benzoborepin, 5,5a,6,10b-tetrahydro-5,6-dimethoxy-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 108946-99-2P 108947-00-8P 108947-01-9P 108947-02-0P
 108947-03-1P 108947-04-2P
 (preparation of)

L12 ANSWER 39 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:439895 HCAPLUS

DOCUMENT NUMBER: 107:39895

TITLE: Contribution to boron chemistry. CLXXV.
 Effect of steric factors on the conformation
 of diborylamines

AUTHOR(S): Maennig, Detlef; Noeth, Heinrich; Prigge,
 Helene; Rotsch, Anne Rose; Gopinathan, Sarada;
 Wilson, J. W.

CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Muenchen, Munich,
 D-8000/2, Fed. Rep. Ger.

SOURCE: Journal of Organometallic Chemistry (1986),
 310(1), 1-20
 CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: German

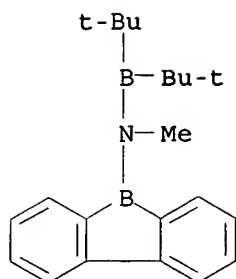
OTHER SOURCE(S): CASREACT 107:39895

AB Ph₂BN(CMe₃)SiMe₃ (I) was prepared from LiN(CMe₃)SiMe₃ and Ph₂BBr, whereas (R₂B)₂NH (II; R = mesityl) and [(R₂B)₂N]₃B (III) were prepared from R₂BNHLi and R₂BF or BF₃.OEt₂, resp.; R₁NMeB(CMe₃)₂ (IV; R₁ = 9-borafluorenyl) was prepared from (Me₃C)₂BNMeLi and R₁Cl. The structures of I-IV, (Ph₂B)₂NH and (Ph₂B)₂NMe were determined by x-ray crystallog. I has a relatively long B-N bond and a nonplanar C₂B-N-CSi skeleton. II and III have a coplanar C₂B-NH-BC₂ (or C₂B-NH-BN₂) unit, whereas (Ph₂B)₂NH and (Ph₂B)₂NMe adopt a twist conformation. IV has an orthogonal conformation, with the (Me₃C)₂B group almost perpendicular to the B-N-C-R₁ plane. Two distinctly different B-N bond lengths are observed. Steric effects on conformation and bonding parameters are discussed.

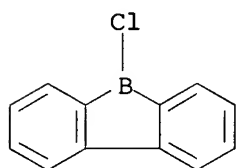
IT 109238-76-8P
 (preparation and crystal and mol. structure of)

RN 109238-76-8 HCAPLUS

CN 5H-Dibenzoborol-5-amine, N-[bis(1,1-dimethylethyl)boryl]-N-methyl-
 (9CI) (CA INDEX NAME)

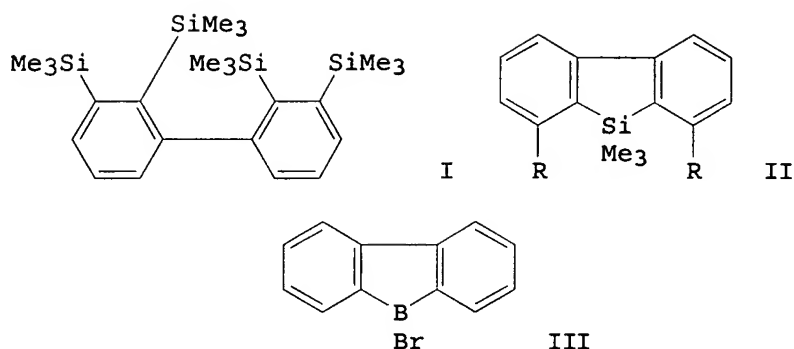


IT 13059-59-1
 (reaction of, with lithium (di-tert-butylboryl)methylamide)
 RN 13059-59-1 HCAPLUS
 CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 109238-73-5P 109238-74-6P 109238-75-7P 109238-76-8P
 (preparation and crystal and mol. structure of)
 IT 13059-59-1
 (reaction of, with lithium (di-tert-butylboryl)methylamide)

L12 ANSWER 40 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1987:423391 HCAPLUS
 DOCUMENT NUMBER: 107:23391
 TITLE: Borylation of arylsilanes. III. Reaction of
 silylated biphenyls and 9H-9-silafluorenes
 with tribromoborane
 AUTHOR(S): Gross, Ulrich; Kaufmann, Dieter
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg,
 D-2000/13, Fed. Rep. Ger.
 SOURCE: Chemische Berichte (1987), 120(6), 991-4
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 107:23391
 GI



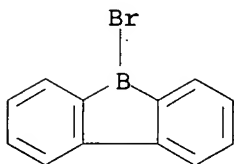
AB The title reactions result either in substitution of a SiMe₃ group by a BBr₂ group or in conversion of a SiMe₃ group to a SiMe₂Br group. Thus, the 1st path occurs with 3- and 4-(trimethylsilyl)biphenyl and 4,4'-bis(trimethylsilyl)biphenyl, whereas the 2nd path predominates with 2-(trimethylsilyl)- and 2,2'-bis(trimethylsilyl)biphenyl. The analogous reaction of tetrasilylated biphenyl I leads first to silafluorene II (R = SiMe₃) and then to dibromo derivative II (R = SiMe₂Br). II (R = H) reacts with BBr₃ to give dibenzoborole III.

IT 97322-60-6P

(preparation of)

RN 97322-60-6 HCAPLUS

CN 5H-Dibenzoborole, 5-bromo- (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 97322-60-6P 107384-79-2P 107384-80-5P,
2-(Dibromoboryl)biphenyl 107384-81-6P, 3-(Dibromoboryl)biphenyl
107384-82-7P, 4-(Dibromoboryl)biphenyl 107384-83-8P,
2,2'-Bis(bromodimethylsilyl)biphenyl 107384-84-9P,
4,4'-Bis(dibromoboryl)biphenyl 107384-85-0P 107384-87-2P
(preparation of)

L12 ANSWER 41 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1986:19613 HCAPLUS

DOCUMENT NUMBER: 104:19613

TITLE: Derivatives of borole. V. Synthesis of
[1-(diisopropylamino)borole]metal complexes
and the Diels-Alder dimer of
1-(diisopropylamino)borole

AUTHOR(S): Herberich, Gerhard E.; Ohst, Holger

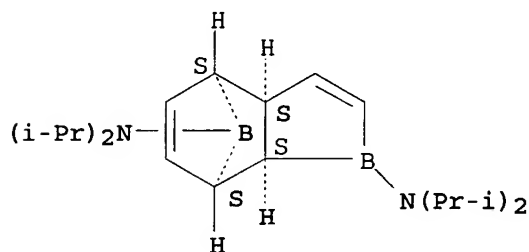
CORPORATE SOURCE: Inst. Anorg. Chem., Tech. Hochsch. Aachen,
Aachen, D-5100, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1985), 118(11), 4303-13
CODEN: CHBEAM; ISSN: 0009-2940

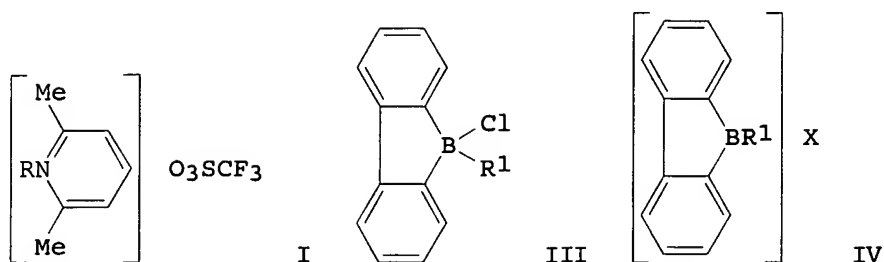
DOCUMENT TYPE: Journal

LANGUAGE: German
 OTHER SOURCE(S): CASREACT 104:19613
 GI For diagram(s), see printed CA Issue.
 AB Oxidation of Li [1-(diisopropylamino)borolenediide] (I) with SnCl₂ forms the Diels-Alder dimer II. I is a versatile reagent for the formation of [1-(diisopropylamino)borole]metal complexes. Suitable substrates are metal halides (CoBr₃·DME, NiCl₂·DME), organometallic metal halides, and simple metal halides in the presence of CO. Thermal reactions of II with carbonyl compds. may also give borole complexes. Fifteen compds. of Cr, Mn, Fe, Co, Ni, Ru, and Rh, including triple-decked complexes, are described.
 IT 99610-64-7P
 (preparation and reaction of, with iron pentacarbonyl)
 RN 99610-64-7 HCAPLUS
 CN 4,7-Borylene-1H-1-benzoborole-1,8-diamine, 3a,4,7,7a-tetrahydro-N,N,N',N'-tetrakis(1-methylethyl)-, (3aα,4α,7α,7α) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 99610-64-7P
 (preparation and reaction of, with iron pentacarbonyl)
 L12 ANSWER 42 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1985:454130 HCAPLUS
 DOCUMENT NUMBER: 103:54130
 TITLE: Contribution to the chemistry of boron. 150. Competition between adduct and cation formation in reactions between diorganylborane derivatives and pyridine or lutidines
 AUTHOR(S): Narula, Chaitanya K.; Noeth, Heinrich
 CORPORATE SOURCE: Inst. Inorg. Chem., Univ. Munich, Munich, D-8000/2, Fed. Rep. Ger.
 SOURCE: Inorganic Chemistry (1985), 24(16), 2532-9
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:54130
 GI



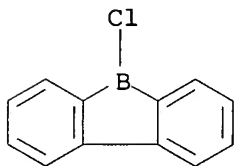
AB 1:1 Coordination compds. are formed in the reaction of pyridine and 2,4-lutidine with $\text{Bu}_2\text{BO}_3\text{SCF}_3$ and 9-[(trifluoromethyl)sulfonyloxy]-9-borabicyclo[3.3.1]nonane and -9-borabicyclo[3.3.1]nonane. In contrast, 2,6-lutidine yields the borenium(1+) triflates (I; R = Bu2B, 9-BBN) with the 1st 2 B triflates. Neutral adducts result from the 3 bases and Bu_2BCl and 9-chloro-9-BBN and -9-borabicyclo[3.3.1]nonane (II), resp. Their interaction with GaCl_3 or AlCl_3 as chloride acceptors leads to N-base exchange in most cases, but GaCl_3 abstrs. Cl^- from II-pyridine III (R_1 = pyridine) to form the red 9-borabicyclo[3.3.1]nonenium tetrachlorogallate IV ($\text{X} = \text{GaCl}_4$), whereas III (R_1 = acridine) and AlCl_3 yield the dark red tetrachloroaluminate IV ($\text{X} = \text{AlCl}_4$) (V). The cation in V shows almost planar acridine and 9-borabicyclo[3.3.1]nonane moieties, whose planes form an angle of 62° . Characteristic for the cation are short B-C bonds (1.35 Å) and a very long C-C single bond (1.66 Å) of the 5-membered borole ring. The formation of base-stabilized diorganylborenium(1+) ions depends on steric and electronic effects.

IT 13059-59-1P

(formation and reaction of, with pyridines)

RN 13059-59-1 HCAPLUS

CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 96806-95-0P 96825-32-0P

(preparation and crystal and mol. structure of)

RN 96806-95-0 HCAPLUS

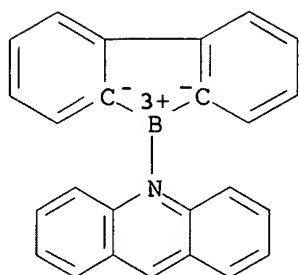
CN Boron(1+), (acridine) [1,1'-biphenyl]-2,2'-diyl-, (T-4)-tetrachloroaluminate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 96806-94-9

CMF C25 H17 B N

CCI CCS

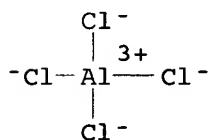


CM 2

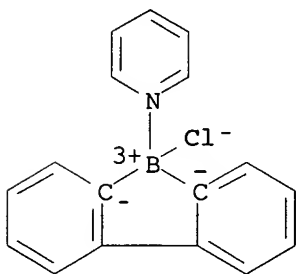
CRN 17611-22-2

CMF Al Cl4

CCI CCS



RN 96825-32-0 HCAPLUS

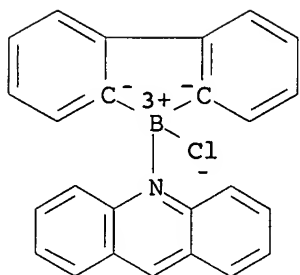
CN Boron, [1,1'-biphenyl]-2,2'-diylchloro(pyridine)-, (T-4)- (9CI)
(CA INDEX NAME)

IT 96806-93-8P

(preparation and reaction of, with aluminum chloride)

RN 96806-93-8 HCAPLUS

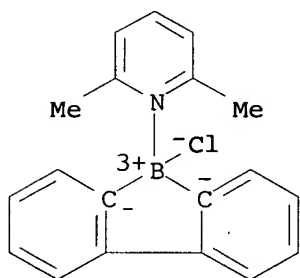
CN Boron, (acridine) [1,1'-biphenyl]-2,2'-diylchloro-, (T-4)- (9CI)
(CA INDEX NAME)



IT 96806-90-5P

(preparation and reaction of, with gallium chloride)

RN 96806-90-5 HCAPLUS

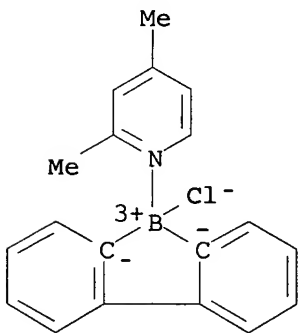
CN Boron, [1,1'-biphenyl]-2,2'-diylchloro(2,6-dimethylpyridine)-,
(T-4)- (9CI) (CA INDEX NAME)

IT 96806-89-2P 96806-92-7P 96806-97-2P

96806-98-3P 96806-99-4P

(preparation of)

RN 96806-89-2 HCAPLUS

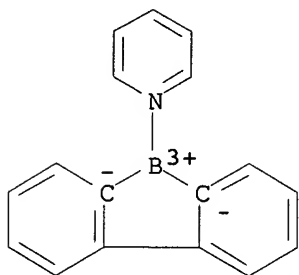
CN Boron, [1,1'-biphenyl]-2,2'-diylchloro(2,4-dimethylpyridine)-,
(T-4)- (9CI) (CA INDEX NAME)

RN 96806-92-7 HCAPLUS

CN Boron(1+), [1,1'-biphenyl]-2,2'-diyl(pyridine)-,
(T-4)-tetrachlorogallate(1-) (9CI) (CA INDEX NAME)

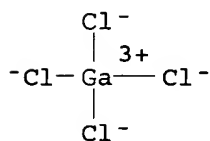
CM 1

CRN 96806-91-6
 CMF C17 H13 B N
 CCI CCS

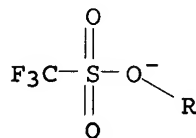
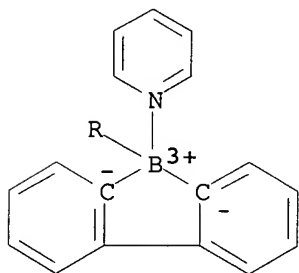


CM 2

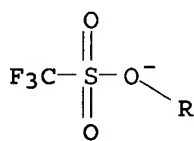
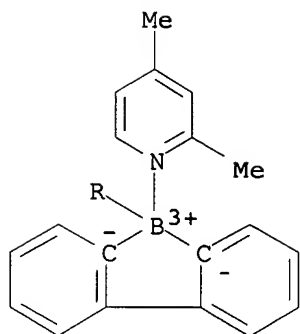
CRN 15201-06-6
 CMF C14 Ga
 CCI CCS



RN 96806-97-2 HCAPLUS
 CN Boron, [1,1'-biphenyl]-2,2'-diyl(pyridine) (trifluoromethanesulfonate-O)-, (T-4)- (9CI) (CA INDEX NAME)

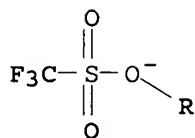
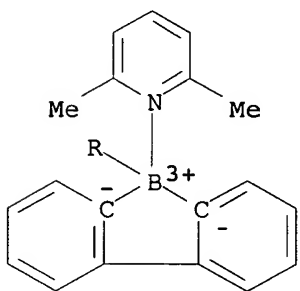


RN 96806-98-3 HCAPLUS
 CN Boron, [1,1'-biphenyl]-2,2'-diyl(2,4-dimethylpyridine) (trifluoromethanesulfonate-O)-, (T-4)- (9CI) (CA INDEX NAME)



RN 96806-99-4 HCAPLUS

CN Boron, [1,1'-biphenyl]-2,2'-diyl(2,6-dimethylpyridine) (trifluoromethanesulfonato-O)-, (T-4)- (9CI) (CA INDEX NAME)

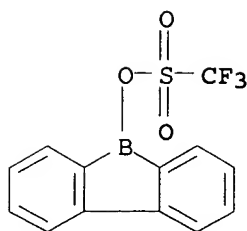


IT 96806-96-1

(reaction of, with pyridines)

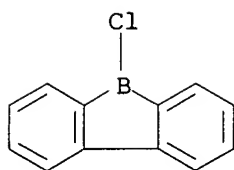
RN 96806-96-1 HCAPLUS

CN 5H-Dibenzoborole, 5-[[trifluoromethylsulfonyl]oxy]- (9CI) (CA INDEX NAME)

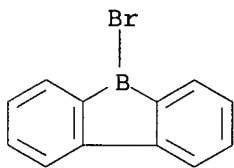


CC 29-4 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 IT 13059-59-1P
 (formation and reaction of, with pyridines)
 IT 96806-95-0P 96825-32-0P
 (preparation and crystal and mol. structure of)
 IT 96806-93-8P
 (preparation and reaction of, with aluminum chloride)
 IT 96806-90-5P
 (preparation and reaction of, with gallium chloride)
 IT 22086-36-8P 96806-77-8P 96806-78-9P 96806-79-0P
 96806-80-3P 96806-81-4P 96806-83-6P 96806-84-7P
 96806-85-8P 96806-86-9P 96806-87-0P 96806-88-1P
 96806-89-2P 96806-92-7P 96806-97-2P
 96806-98-3P 96806-99-4P 96807-01-1P
 96807-02-2P 96807-03-3P
 (preparation of)
 IT 1730-69-4 22086-34-6 60669-69-4 62731-43-5
 96806-96-1
 (reaction of, with pyridines)

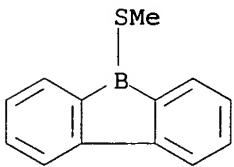
L12 ANSWER 43 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1985:454126 HCAPLUS
 DOCUMENT NUMBER: 103:54126
 TITLE: Contributions to the chemistry of boron.
 CLVI. A convenient route to 9-borfluorenes
 AUTHOR(S): Narula, Chaitanya K.; Noeth, Heinrich
 CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Muenchen, Munich,
 8000/2, Fed. Rep. Ger.
 SOURCE: Journal of Organometallic Chemistry (1985),
 281(2-3), 131-4
 CODEN: JORCAI; ISSN: 0022-328X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:54126
 AB A convenient high yield synthesis is reported for
 9-halo-9-borfluorene from o,o'-mercurated di-Ph and boron
 halides. These in turn are easily converted into methoxy-, and
 methylthio- and diethylamino derivs.
 IT 13059-59-1P
 (preparation and amine substitution of)
 RN 13059-59-1 HCAPLUS
 CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



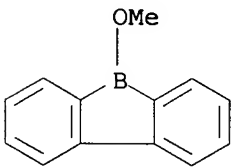
IT 97322-60-6P
(preparation and methoxy substitution of)
RN 97322-60-6 HCAPLUS
CN 5H-Dibenzoborole, 5-bromo- (9CI) (CA INDEX NAME)



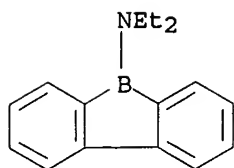
IT 97322-61-7P 97322-62-8P 97322-63-9P
97341-63-4P 97348-78-2P
(preparation of)
RN 97322-61-7 HCAPLUS
CN 5H-Dibenzoborole, 5-(methylthio)- (9CI) (CA INDEX NAME)



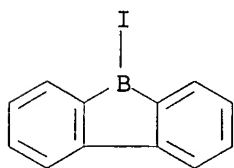
RN 97322-62-8 HCAPLUS
CN 5H-Dibenzoborole, 5-methoxy- (9CI) (CA INDEX NAME)



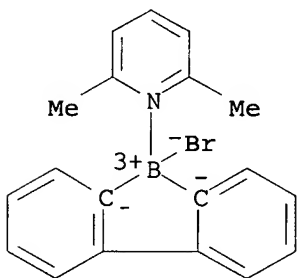
RN 97322-63-9 HCAPLUS
CN 5H-Dibenzoborol-5-amine, N,N-diethyl- (9CI) (CA INDEX NAME)



RN 97341-63-4 HCAPLUS
 CN 5H-Dibenzoborole, 5-iodo- (9CI) (CA INDEX NAME)



RN 97348-78-2 HCAPLUS
 CN Boron, [1,1'-biphenyl]-2,2'-diylbromo(2,6-dimethylpyridine)-, (T-4)- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 13059-59-1P
 (preparation and amine substitution of)
 IT 97322-60-6P
 (preparation and methoxy substitution of)
 IT 97322-61-7P 97322-62-8P 97322-63-9P
 97341-63-4P 97348-78-2P
 (preparation of)

L12 ANSWER 44 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:629850 HCAPLUS

DOCUMENT NUMBER: 101:229850

TITLE: Ions. 13. Understanding the concepts
 enantiomer and enantiotope

AUTHOR(S): Schiemenz, Gunter P.; Pistor, Johann

CORPORATE SOURCE: Inst. Org. Chem., Univ. Kiel, Kiel, D-2300,
 Fed. Rep. Ger.

SOURCE: Chemica Scripta (1984), 23(5), 216-23

CODEN: CSRPB9; ISSN: 0004-2056

DOCUMENT TYPE: Journal

LANGUAGE: German

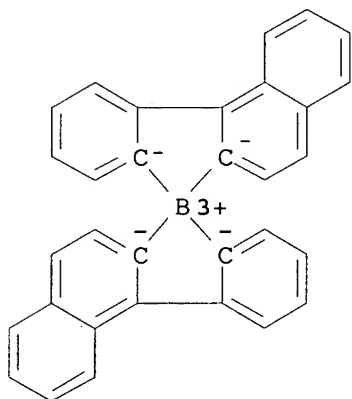
AB The ¹H NMR spectra of chiral sulfonium hexaarylphosphates reveal

that enantiotopism is not a property but an intellectual concept, the conditions of which are never strictly met. Enantiotopic groups are, in fact, diastereotopic. Likewise, enantiomeric compds. do not represent a stereochem. category of their own, but only a special case of diastereomerism. The essential point of enantiotopic groups and enantiomeric compds. is not their similarity but the difference between them.

IT 93303-64-1
(NMR of)
RN 93303-64-1 HCAPLUS
CN Sulfonium, [2,5-bis(1-methylethyl)phenyl]dimethyl-,
(T-4)-(-)-bis(2,1-naphthalenediyl-1,2-phenylene)borate(1-) (9CI)
(CA INDEX NAME)

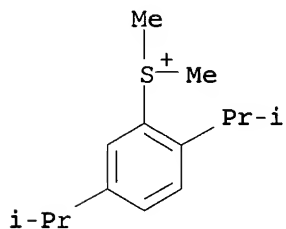
CM 1

CRN 93303-63-0
CMF C32 H20 B
CCI CCS



CM 2

CRN 93251-82-2
CMF C14 H23 S

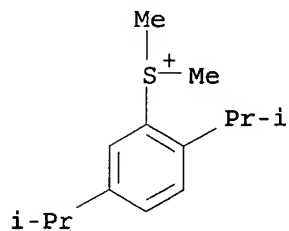


IT 93251-85-5
(NMR of racemic)
RN 93251-85-5 HCAPLUS
CN Sulfonium, [2,5-bis(1-methylethyl)phenyl]dimethyl-,
(T-4)-bis(2,1-naphthalenediyl-1,2-phenylene)borate(1-) (9CI) (CA
INDEX NAME)

CM 1

CRN 93251-82-2

CMF C14 H23 S

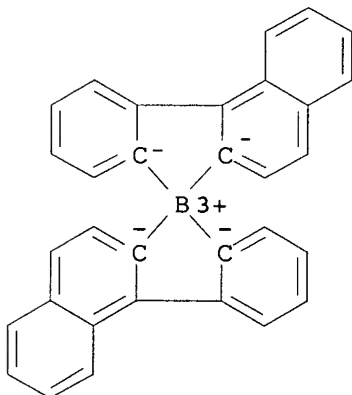


CM 2

CRN 3275-39-6

CMF C32 H20 B

CCI CCS



CC 22-10 (Physical Organic Chemistry)

IT 93251-83-3 93251-84-4 93251-86-6 93251-87-7 93251-88-8

93303-64-1

(NMR of)

IT 93251-85-5 93274-15-8

(NMR of racemic)

L12 ANSWER 45 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:571316 HCAPLUS

DOCUMENT NUMBER: 101:171316

TITLE: Compounds of pentacoordinate (10-B-5) and hexacoordinate (12-B-6) hypervalent boron

AUTHOR(S): Lee, David Y.; Martin, J. C.

CORPORATE SOURCE: Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA

SOURCE: Journal of the American Chemical Society (1984), 106(19), 5745-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

AB Syntheses of the 1st isolable hypervalent 10-B-5 species I, II and III, and of 12-B-6 species IV are described. The ^1H , ^{13}C and ^{19}F NMR spectra support the assigned hypervalent structures. The UV-visible spectrum of I shows an absorption maximum (397 nm, $\epsilon = 1650$) which is consistent with delocalization of the electrons of the electron-rich, 3-center hypervalent bond into the π -acceptor 5-membered ring. This makes the π system a 6-electron, Hückel bis-ipso aromatic species.

IT 91898-98-5P

(preparation and reaction of, with triflic acid)

RN 91898-98-5 HCAPLUS

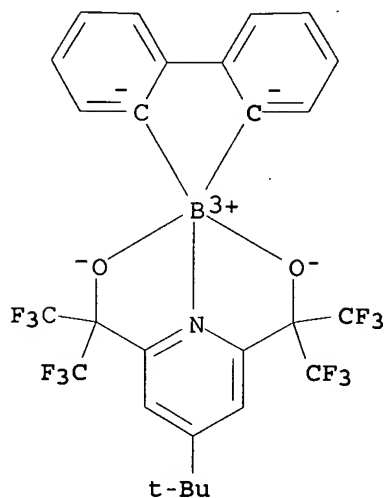
CN Ethanaminium, N,N,N-triethyl-, (TB-5-11)-[1,1'-biphenyl]-2,2'-diyl[4-(1,1-dimethylethyl)- $\alpha,\alpha,\alpha',\alpha'$ -tetrakis(trifluoromethyl)-2,6-pyridinedimethanolato(2-)-N1, $O\alpha,O\alpha'$]borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 91898-97-4

CMF C27 H19 B F12 N O2

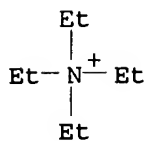
CCI CCS



CM 2

CRN 66-40-0

CMF C8 H20 N

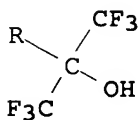
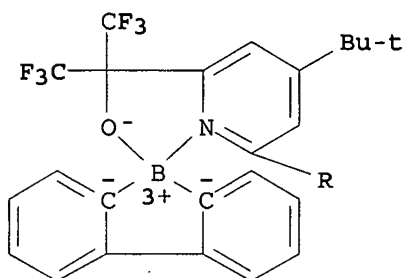


IT 91898-99-6P

(preparation of)

RN 91898-99-6 HCAPLUS

CN Boron, [1,1'-biphenyl]-2,2'-diyl[4-(1,1-dimethylethyl)-
 $\alpha,\alpha,\alpha',\alpha'$ -tetrakis(trifluoromethyl)-2,6-
 pyridinedimethanolato-N1,O α]-, (T-4)- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

IT 91898-98-5P 91899-05-7P

(preparation and reaction of, with triflic acid)

IT 91898-99-6P 91899-02-4P 91899-03-5P 91899-06-8P

(preparation of)

L12 ANSWER 46 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:191923 HCAPLUS

DOCUMENT NUMBER: 100:191923

TITLE: The reaction of methylborylene with
 cyclohexene and some other olefinic compounds
 AUTHOR(S): Van der Kerk, S. M.; Roos-Venekamp, J. C.; Van
 Beijnen, A. J. M.; Van der Kerk, G. J. M.

CORPORATE SOURCE: Lab. Org. Chem., State Univ. Utrecht, Utrecht,
 3522 AD, Neth.

SOURCE: Polyhedron (1983), 2(12), 1337-43
 CODEN: PLYHDE; ISSN: 0277-5387

DOCUMENT TYPE: Journal

LANGUAGE: English

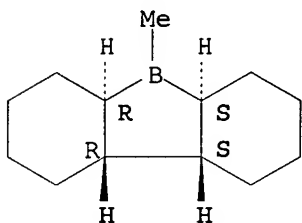
OTHER SOURCE(S): CASREACT 100:191923

AB Some potential methylborylene-generating systems were
 investigated, using cyclohexene as the trapping agent.
 Methylborylene, generated by the system 2C8K/MeBBr₂, reacts with
 cyclohexene to yield 2-methyl-2-boratricyclo[7.4.0.0^{3,8}]tridecane
 (I). An isomer of I was synthesized along a completely different

route. With the system 2C8K/MeBBr₂, only cyclic olefins were converted to analogs of I. An acyclic olefin and a conjugated diene yielded only haloboration products. Possible mechanisms leading to the formation of I are discussed. The system NaK5/MeBBr₂ led to explosion.

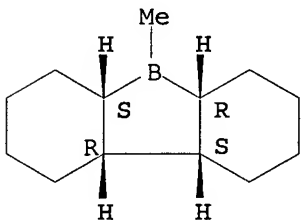
IT 89920-47-8P
(preparation and spectra of)
RN 89920-47-8 HCAPLUS
CN 1H-Dibenzoborole, dodecahydro-5-methyl-,
(4a α ,5a α ,9a β ,9b β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 89920-46-7
(separation, spectra, and reaction with ethyllithium)
RN 89920-46-7 HCAPLUS
CN 1H-Dibenzoborole, dodecahydro-5-methyl-,
(4a α ,5a α ,9a α ,9b α) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 29-4 (Organometallic and Organometalloidal Compounds)
IT 89920-47-8P
(preparation and spectra of)
IT 89920-46-7
(separation, spectra, and reaction with ethyllithium)

L12 ANSWER 47 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:15869 HCAPLUS
DOCUMENT NUMBER: 94:15869
TITLE: Ether adducts of organic-alkali metal-boron salts
INVENTOR(S): Klemann, Lawrence P.; Stogryn, Eugene L.
PATENT ASSIGNEE(S): Exxon Research and Engineering Co., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4224256	A	19800923	US 1979-34578	1979 0430

PRIORITY APPLN. INFO.: <-- US 1979-34578 A 1979 0430

AB NH₄⁺ BPh₄⁻ (17.2 g) was refluxed 4 h with 1.6 g LiH in 80 mL dioxolane to give 22.8 g L₄Li⁺ BPh₄⁻ (L = dioxolane). Similarly prepared were 10 L₄Li⁺ BR₄⁻ (L = dioxolane, Et₂O, MeOCH₂CH₂OMe; R = p- and m-CF₃CH₂H₄, p-FC₆H₄, 2-thienyl).

IT 75964-84-0P (preparation of)

RN 75964-84-0 HCAPLUS

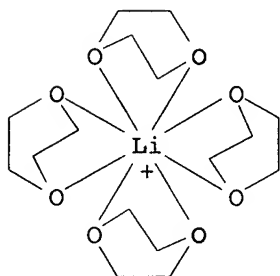
CN Lithium(1+), tetrakis(1,4-dioxane-01,04)-, (T-4)-bis([1,1'-biphenyl]-2,2'-diyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 75964-71-5

CMF C16 H32 Li O8

CCI CCS

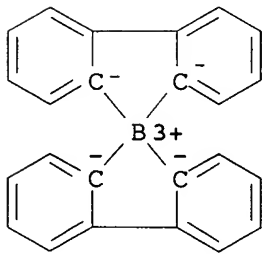


CM 2

CRN 35861-06-4

CMF C24 H16 B

CCI CCS



IC C07F005-02
 INCL 568006000
 CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 75964-72-6P 75964-73-7P 75964-75-9P 75964-76-0P
 75964-77-1P 75964-79-3P 75964-80-6P 75964-82-8P
 75964-83-9P 75964-84-0P 75965-35-4P 75978-35-7P
 (preparation of)

L12 ANSWER 48 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:471920 HCAPLUS

DOCUMENT NUMBER: 93:71920

TITLE: Photoinsertion of alkynes into a ferraborane.
 Preparation and characterization of a novel
 tetracarbon carborane

AUTHOR(S): Fehlner, Thomas P.

CORPORATE SOURCE: Dep. Chem., Univ. Notre Dame, Notre Dame, IN,
 46556, USA

SOURCE: Journal of the American Chemical Society
 (1980), 102(10), 3424-30
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

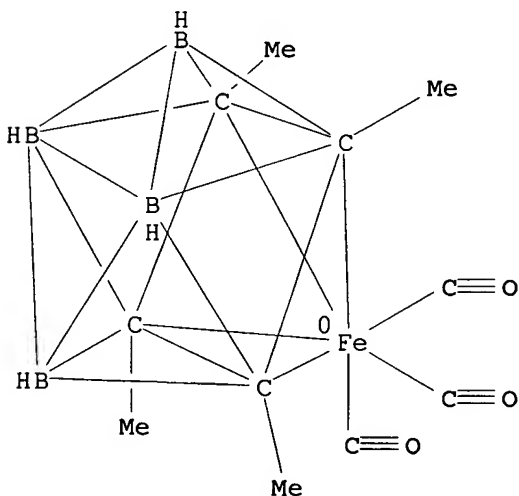
LANGUAGE: English

AB Photolysis of the nido ferraborane $B_4H_8Fe(CO)_3$ and an alkyne
 $RC.tplbond.CR$ ($R = Me, Ph$) gave good yields of tetracarbon
 carboranes $R_4C_4B_4H_4$. The C-tetra-Me derivative was characterized
 primarily by mass and NMR spectroscopy. An intermediate in the
 formation of this carborane, $Me_4C_4B_4H_4Fe(CO)_3$, was isolated and
 partially characterized. Six- and eight-carbon carboranes were
 also likely in this system. In contrast, the isoelectronic
 cyclobutadienyliron compound $C_4H_4Fe(CO)_3$ gives benzenes when
 photolyzed with alkynes.

IT 74469-65-1P
 (preparation of)

RN 74469-65-1 HCAPLUS

CN Iron, tricarbonyl[η^4 -tetrahydro-C,C',C'',C'''-
 tetramethyltetracarbaoctaborato(2-)]- (9CI) (CA INDEX NAME)

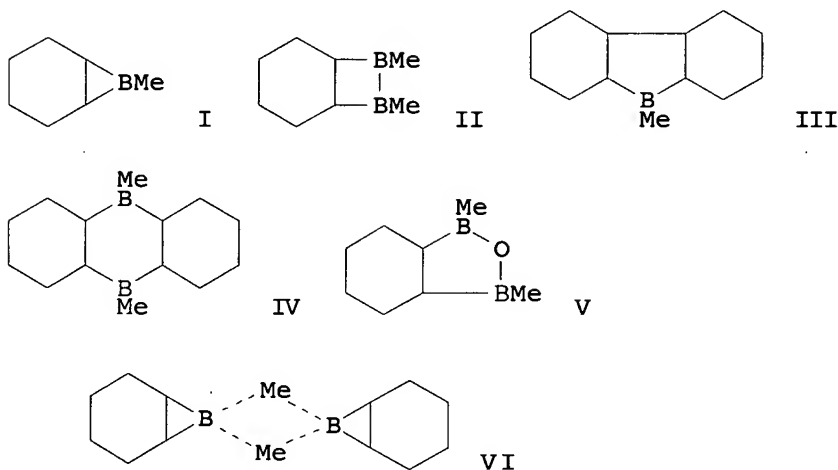


CC 29-12 (Organometallic and Organometalloidal Compounds)
 IT 74417-78-0P 74417-79-1P 74417-80-4P 74453-94-4P

74469-65-1P

(preparation of)

L12 ANSWER 49 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1977:190050 HCAPLUS
 DOCUMENT NUMBER: 86:190050
 TITLE: The generation and some reactions of methylborylene
 AUTHOR(S): Van der Kerk, S. M.; Boersma, J.; Van der Kerk, G. J. M.
 CORPORATE SOURCE: Lab. Org. Chem., State Univ., Utrecht, Neth.
 SOURCE: Tetrahedron Letters (1976), (51), 4765-6
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



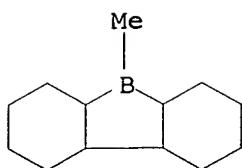
AB MeB:, generated from MeBBr₂ and NaK₅, reacted with cyclohexene to give, on the basis of gas chromatog. and mass spectral anal., the reaction products I-V. Reaction of MeB:, generated from MeBBr₂ and C₈K, with cyclohexene gave only MeBBr₂ and a compound having the formula C₇H₁₃B (I). Further gas chromatog. and mass spectral anal. showed the compound to exist as the dimer VI rather than the monomer I and represents the first example of a simple B-C compound in which B has attained tetracoordination by means of forming two boron-carbon two electron-three center bonds.

IT 62785-44-8P

(preparation of)

RN 62785-44-8 HCAPLUS

CN 1H-Dibenzoborole, dodecahydro-5-methyl- (9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 62785-42-6P 62785-43-7P 62785-44-8P 62785-45-9P
 62785-46-0P
 (preparation of)

L12 ANSWER 50 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:111419 HCAPLUS

DOCUMENT NUMBER: 82:111419

TITLE: Organic quantum chemistry. XXXIII.
 Electronic spectra and rotational barriers of
 vinylborane, allyl cation, and related
 compounds

AUTHOR(S): Allinger, Norman L.; Siefert, John H.
 CORPORATE SOURCE: Dep. Chem., Univ. Georgia, Athens, GA, USA
 SOURCE: Journal of the American Chemical Society

(1975), 97(4), 752-60

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

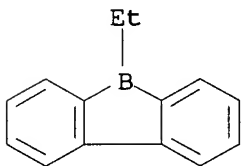
AB The geometrics of the ground states and the rotational barriers
 were studied for vinylborane (I) and di- and trivinylboranes by
 the INDO method. For I, ab initio calcns. were also carried out.
 Using these geometries, the variable electronegativity SCF method
 for the π system was developed so that after configuration
 interaction, including all singly and doubly excited
 configurations, calcns. of the electronic spectra were possible.
 These calcns. were applied to more complicated unsatd. B derivs.
 Similar studies on the related allyl ions were briefly mentioned.
 The calculated spectra show large systematic errors, believed due
 mainly to hyperconjugation, which was not taken into account.

IT 14855-16-4

(UV spectrum of, MO calcn. of)

RN 14855-16-4 HCAPLUS

CN 5H-Dibenzoborole, 5-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)

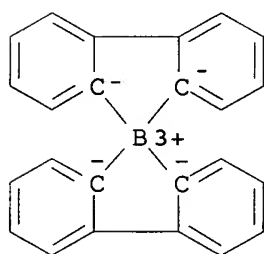
IT 287-87-6 14855-16-4 16703-13-2 54963-15-4
 54963-16-5 54963-17-6 54963-18-7

(UV spectrum of, MO calcn. of)

L12 ANSWER 51 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:111284 HCAPLUS

DOCUMENT NUMBER: 82:111284
 TITLE: Rearrangements of organometallic compounds.
 XII. Generation of boracarbenoid and boracyclopropene intermediates from the photolysis of tetraorganoborate salts in aprotic media
 AUTHOR(S): Eisch, John J.; Tamao, Kohei; Wilcsek, Robert J.
 CORPORATE SOURCE: Dep. Chem., State Univ. New York, Binghamton, NY, USA
 SOURCE: Journal of the American Chemical Society (1975), 97(4), 895-7
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Irradiation of NaBPh₄ in MeOCH₂CH₂OMe and THF, under nitrogen led to two photoreactions: a) the principal one yielding, directly, PhPh and NaBPh₂; and b) the minor one, involving the formation of sodium arylborohydrides, where the aryl group was phenyl, biphenyl, m-terphenyl or p-terphenyl. NaBPh₂ was characterized chemically by its treatment with DOAc to generate D₂ and by its carbene-like addition to PhC.tplbond.CPh to yield, after deuterolytic work-up, deuterated cis-stilbenes. The reaction with PhC.tplbond.CPh caused the transitory generation of the boracyclopropene nucleus as the diphenyl-(diphenylvinylene)borate(III) salt. This was substantiated by a highly selective and stereospecific 1,2-phenyl shift in the photorearrangement of LiBPh₃(C.tplbond.CPh). Examination of the analogous photolytic behavior of other tetraorganoborate salts established the geometrical constraints and intraionic character of the biaryl formation in the principal photoreaction.
 IT 54873-17-5
 (photochem. reaction of)
 RN 54873-17-5 HCAPLUS
 CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, sodium, (T-4)- (9CI)
 (CA INDEX NAME)

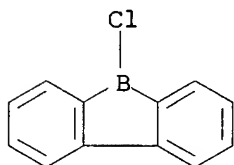


● Na⁺

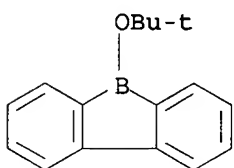
CC 22-4 (Physical Organic Chemistry)
 IT 54873-15-3 54873-16-4 54873-17-5
 (photochem. reaction of)

L12 ANSWER 52 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1975:86313 HCAPLUS

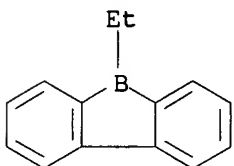
DOCUMENT NUMBER: 82:86313
TITLE: Boron compounds. XXVIII.
1,2-(2,2'-Biphenylylene)diboranes(6)
AUTHOR(S): Koester, Roland; Willemsen, Hans G.
CORPORATE SOURCE: Max-Planck-Inst. Kohlenforsch., Muelheim/Ruhr,
Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (1975),
Volume Date 1974, (11), 1843-50
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Reaction of 2-biphenylyldiethylborane and ethyldiborane(6) gave
.apprx.80% 1,2-diethyl-1,2-(2,2'-biphenylylene)diborane(6) (I).
Reaction of I with B₂H₆ and BF₃.Et₂O gave 1,2-(2,2'-
biphenylylene)diborane-(6) and 1,2;1,2-bis(2,2'-
biphenylylene)diborane(6), resp. Reaction of I with Me₃COH and BCl₃
gave colorless 9-tert-butoxy-9-borafluorene and yellow
9-chloro-9-borafluorene, resp.
IT 13059-59-1P
(preparation and salt formation from)
RN 13059-59-1 HCAPLUS
CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 55365-17-8P
(preparation of)
RN 55365-17-8 HCAPLUS
CN 5H-Dibenzoborole, 5-(1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)



IT 14855-16-4
(reaction with ethyldiborane)
RN 14855-16-4 HCAPLUS
CN 5H-Dibenzoborole, 5-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)
 IT 13059-59-1P
 (preparation and salt formation from)
 IT 55365-17-8P 55802-26-1P 55802-27-2P
 (preparation of)
 IT 14855-16-4
 (reaction with ethyldiborane)

L12 ANSWER 53 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:72416 HCAPLUS

DOCUMENT NUMBER: 82:72416

TITLE: Expanded Hueckel calculation of hypothetical systems. Carbododecahedron (C20) and different diboracarbododecahedrons (B2C18)

AUTHOR(S): Bochvar, D. A.; Gal'pern, E. G.

CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya

Khimicheskaya (1974), (10), 2367-9

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Russian

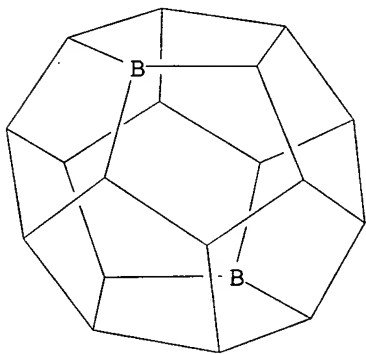
AB Title calcns. for (hypothetical) carbododecahedron (C20) and 1,2- and 1,6-diboracarbododecahedrons indicated that they are capable of existence.

IT 54350-39-9 54350-40-2

(MO calcns. for)

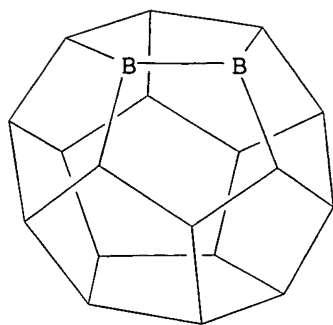
RN 54350-39-9 HCAPLUS

CN 1,20-Dibora[5]fullerane-C20-Ih (9CI) (CA INDEX NAME)



RN 54350-40-2 HCAPLUS

CN 5,2,1,6,3,4-[2,3]Butanediyl[1,4]diylidenecyclopenta[3',4']pentalen
 o[6',1',2':2,3,4]pentaleno[1,6-cd]-1,2-diborole, tetradecahydro-
 (9CI) (CA INDEX NAME)



CC 22-8 (Physical Organic Chemistry)
 IT 4493-23-6 54350-39-9 54350-40-2
 (MO calcns. for)

L12 ANSWER 54 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:42485 HCAPLUS

DOCUMENT NUMBER: 82:42485

TITLE: NMR studies of boron compounds. VIII.
 Comparison of boron-11 and nitrogen-14 NMR
 data of tricoordinate boron compounds with
 carbon-13 and nitrogen-14 NMR data of carbonic
 acid derivatives and carbonium ions

AUTHOR(S): Noeth, Heinrich; Wrackmeyer, Bernd
 CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Muenchen, Munich,
 Fed. Rep. Ger.

SOURCE: Chemische Berichte (1974), 107(9), 3089-103
 CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

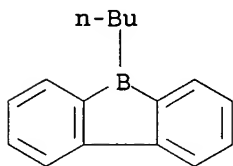
LANGUAGE: German

AB A comparison of ^{11}B -, ^{14}N -, and ^{13}C -NMR data revealed a linear
 relation between the ^{14}N shifts of aminoboranes, e.g., $\text{B}(\text{NMe}_2)_3$ or
 Me_2BNMe_2 , and isoelectronic and(or) isosteric (aliphatic or
 heterocyclic) amines or ammonium ions.

IT 7760-71-6
 (boron-11 NMR of)

RN 7760-71-6 HCAPLUS

CN 5H-Dibenzoborole, 5-butyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)

IT 121-43-7 353-46-8 593-90-8 960-71-4 1803-36-7 4443-43-0

4542-61-4 5158-50-9 5846-37-7 7216-97-9 7318-81-2

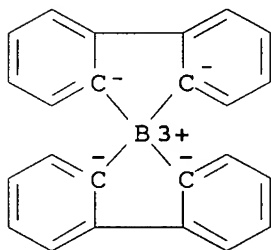
7760-71-6 12538-96-4 13283-31-3, properties

15909-61-2 19163-04-3 19163-14-5 19163-15-6 22405-02-3

54098-91-8 54098-92-9 54098-93-0 54098-94-1 54228-72-7

(boron-11 NMR of)

L12 ANSWER 55 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1974:437022 HCAPLUS
 DOCUMENT NUMBER: 81:37022
 TITLE: Rearrangements of organometallic compounds.
 XI. Duality of mechanism for 1,2-aryl
 migrations in the oxidation of tetraarylborate
 salts
 AUTHOR(S): Eisch, John J.; Wilcsek, Robert J.
 CORPORATE SOURCE: Dep. Chem., State Univ. New York, Binghamton,
 NY, USA
 SOURCE: Journal of Organometallic Chemistry (1974),
 71(2), C21-C24
 CODEN: JORCAI; ISSN: 0022-328X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Individual oxidative couplings of K phenyltri-m-tolylborate and K
 phenyltri-p-tolylborate with transition metal ions, organic oxidants
 and halogen sources revealed a duality of mechanism, namely
 electron-transfer and electrophilic pathways. Not only the ratios
 of the resp. bitolyls and methylbiphenyls obtained, but also the
 behavior of K bis(o,o'-biphenylene)borate, showed
 that bridging of the migrating group is important for iodine
 oxidns., but not for Ce(IV) oxidns.
 IT 53113-49-8
 (oxidation of)
 RN 53113-49-8 HCAPLUS
 CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, potassium, (T-4)-
 (9CI) (CA INDEX NAME)



● K⁺

CC 22-5 (Physical Organic Chemistry)
 IT 53113-49-8
 (oxidation of)

L12 ANSWER 56 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1973:58494 HCAPLUS
 DOCUMENT NUMBER: 78:58494
 TITLE: Synthesis of 5- and 6-membered carbon-boron
 heterocycles by pyrolysis of
 pyridine-arylboranes
 AUTHOR(S): Van Veen, R.; Bickelhaupt, F.
 CORPORATE SOURCE: Scheikundig Lab., Vrije Univ., Amsterdam,
 Neth.
 SOURCE: Journal of Organometallic Chemistry (1973),

47(1), 33-8

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE:

Journal

LANGUAGE:

English

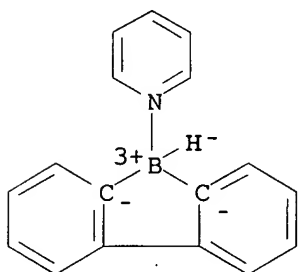
AB Pyrolysis of pyridine(2-benzylphenyl)borane and pyridine(2-benzhydrylphenyl)borane yielded the 9,10-dihydro-9-boraanthracene system. The ring-closed products were isolated as the ethanolamine esters. An analogous conversion of pyridine-2-biphenylborane gave pyridine-9-borafluorene.

IT 40374-82-1P

(preparation of)

RN 40374-82-1 HCAPLUS

CN Boron, [1,1'-biphenyl]-2,2'-diylhydro(pyridine)-, (T-4)- (9CI)
(CA INDEX NAME)



CC 29-4 (Organometallic and Organometalloidal Compounds)

IT 7147-07-1P 28776-05-8P 40276-63-9P 40276-64-0P 40276-66-2P

40374-82-1P 40374-83-2P 40374-84-3P

(preparation of)

L12 ANSWER 57 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:427134 HCAPLUS

DOCUMENT NUMBER: 77:27134

TITLE: Dynamics of intramolecular triplet exciton transfer using electron spin resonance

AUTHOR(S): Shain, Albert L.

CORPORATE SOURCE: Dep. Chem., Washington Univ., St. Louis, MO, USA

SOURCE: Journal of Chemical Physics (1972), 56(12), 6201-12

CODEN: JCPSA6; ISSN: 0021-9606

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The rate of intramol. triplet exciton transfer in a series of congeneric dimeric systems composed of 2 biphenylene subunits linked by an insulating tetravalent Group IVA atom was studied as a function of temperature using ESR. A 1st-order d. matrix theory including the transfer process was developed. The transfer model assumed a coupling between the "high-field" monomer magnetic substrates with the same m5 only (T2 process), without inducing transitions between states of different m3 (T1 processes). By comparing computer simulated line shapes with the exptl. spectra, activation energies for the dynamic process were extracted. These energies are attributed to low-frequency torsional modes which are active in vibronically coupling the monomer sites. A discussion based on electron exchange and on vibronic coupling is given, and an order of magnitude calcn. of the transfer

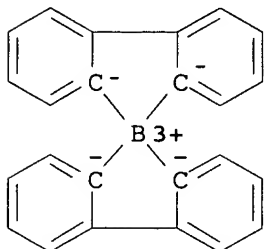
probability based on the resonance excitation transfer mechanism yields nos. agreeing satisfactorily with the transfer rates obtained from experiment

IT 25360-44-5

(ESR of, intramol. triplet exciton transfer dynamics in relation to)

RN 25360-44-5 HCAPLUS

CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, cesium, (T-4)- (9CI)
(CA INDEX NAME)



● Cs⁺

CC 73-4 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)

Section cross-reference(s): 22

IT 86-73-7 159-66-0 159-67-1 159-68-2 3151-19-7 5550-08-3
25105-80-0 25360-44-5 37020-91-0

(ESR of, intramol. triplet exciton transfer dynamics in relation to)

L12 ANSWER 58 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:492904 HCAPLUS

DOCUMENT NUMBER: 73:92904

TITLE: Calculation of excited state and ground state properties of conjugated heteroatomic molecules using a single SCF-LCAO-CI method including σ -polarization

AUTHOR(S): Hammond, Howell A.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA

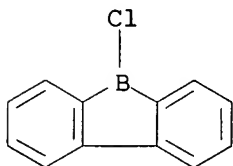
SOURCE: Theoretica Chimica Acta (1970), 18(3), 239-49
CODEN: TCHAAM; ISSN: 0040-5744

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An SCF- π method including variable π -electronegativity and σ -polarization is described and applied to the calcn. of electronic transitions and ionization potentials of a large variety of heteroat. mols. containing B, N, O, F, Cl, and S. The necessary atomic parameters are the Slater effective nuclear charges and published ionization potentials, electron affinities and σ -orbital electronegativities for trigonally hybridized atoms. The program automatically adjusts the initial atomic parameters to reflect the mol. environment without the intervention of the user. The agreement between calculated and observed transition energies, oscillator strengths, and ionization

potentials is very good.
 IT 13059-59-1
 (mol. orbitals of, mol. consts. in relation to)
 RN 13059-59-1 HCAPLUS
 CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
 IT 91-58-7 98-80-6 98-95-3, properties 100-47-0 106-51-4, properties 108-95-2, properties 271-89-6 273-53-0 486-25-9 873-51-8 2622-57-3 13059-59-1 16969-45-2, properties (mol. orbitals of, mol. consts. in relation to)

L12 ANSWER 59 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:121610 HCAPLUS

DOCUMENT NUMBER: 72:121610

TITLE: Boron containing analog of the norbornene ring system

AUTHOR(S): Grisdale, Patrick J.; Williams, Jack L. R.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA

SOURCE: Journal of Organometallic Chemistry (1970), 22(2), C19-C21

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tetramethylammonium 1,1,2,3,4,5-hexaphenylborolate (I), m. 227-30°, was prepared (yield 70%) from LiCPh:CPHCPH:CPhLi with Ph₂BCl and Me₄NBr. I undergoes facile Diels-Alder reaction with π -electron-poor dienophiles. Thus, I reacts with maleic anhydride in Me₂CO to give tetramethylammonium 1,4,5,6,7,7-hexaphenyl-7-boratobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic anhydride, m. 185° (decomposition). Similarly, N-phenyl and N-(α -pyridyl)-maleimide react with I to give Diels-Alder adducts. The compds. were characterized by ir, NMR, and mass spectra.

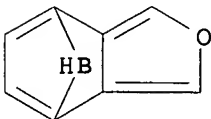
IT 27301-27-5DP, 4,7-Boryleneisobenzofuran, derivs.

28627-98-7P

(preparation of)

RN 27301-27-5 HCAPLUS

CN 4,7-Boryleneisobenzofuran (8CI, 9CI) (CA INDEX NAME)



RN 28627-98-7 HCAPLUS

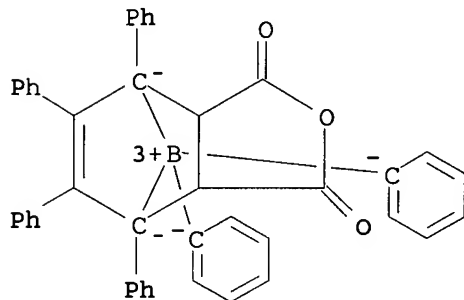
CN Ammonium, tetramethyl-, (5,6-dicarboxy-1,2,3,4-tetraphenyl-2-cyclohexen-1,4-ylene)diphenylborate(1-), cyclic anhydride (8CI)
(CA INDEX NAME)

CM 1

CRN 47868-73-5

CMF C44 H32 B O3

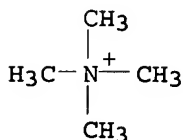
CCI CCS



CM 2

CRN 51-92-3

CMF C4 H12 N



CC 29 (Organometallic and Organometalloidal Compounds)
IT 806-71-3DP, 1,3-Butadiene, 1,2,3,4-tetraphenyl-, boron complexes
27301-26-4DP, 7-Borabicyclo[2.2.1]heptane, derivs.
27301-27-5DP, 4,7-Boryleneisobenzofuran, derivs.
28627-97-6P 28627-98-7P
(preparation of)

L12 ANSWER 60 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:523312 HCAPLUS

DOCUMENT NUMBER: 71:123312

TITLE: Intramolecular triplet exciton transfer in
some noncoplanar aromatic systems

AUTHOR(S): Shain, Albert L.; Ackerman, J. P.; Teague, M.
Warfield

CORPORATE SOURCE: Washington Univ., St. Louis, MO, USA

SOURCE: Chemical Physics Letters (1969), 3(7), 550-1
CODEN: CHPLBC; ISSN: 0009-2614

DOCUMENT TYPE: Journal

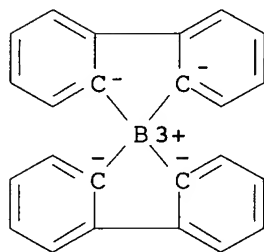
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB E.S.R. spectra were recorded of the lowest triplet state of some
noncoplanar bis(2,2'-biphenylene)spirans (I) at

4.2-200°K. Spectra of I [M = C, B-(Cs+), or N+(Br-)] indicate intramol. migration of triplet exciton transfer (at a rate of $\geq 1.5 \times 10^9$ sec.⁻¹ at 77°K. for M = C). At 18°K., the triplet exciton is localized in one of the biphenylene subunits and the spectrum is characteristic of a system with C_{2v} symmetry (E = 29 gauss). At 77°K., the exciton transfers rapidly between the 2 biphenylylenes and the spectrum becomes characteristic of the whole mol. of D_{2d} symmetry (E = 0). For I (M = C), a single rate constant describes the temperature dependence between 20 and 40°K. and indicates an activation energy of .apprx.100 cal./mole; from 40 to 60°K., the activation energy is .apprx.300 cal./mole. These activation energies correspond to low frequency torsional motions of .apprx.35 and 100 cm.⁻¹ E.S.R. spectra of I (M = Si or Ge) are essentially temperature independent and are characteristic of nonaxially sym., and axially sym. systems, resp. The differences in spectra of the latter 2 compds. are due to the vacant d-orbitals on the spiro atoms.

IT 25360-44-5
(energy transfer in excited mols. of)
RN 25360-44-5 HCAPLUS
CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, cesium, (T-4)- (9CI)
(CA INDEX NAME)



● Cs⁺

CC 22 (Physical Organic Chemistry)
IT 159-66-0 159-67-1 159-68-2 25105-80-0 25360-44-5
(energy transfer in excited mols. of)

L12 ANSWER 61 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:68452 HCAPLUS
DOCUMENT NUMBER: 70:68452
TITLE: Boron compounds. XVI. Haloorganoboranes by catalytic disproportionation of trihaloboranes and organoboranes
AUTHOR(S): Koester, Roland; Grassberger, Maximilian A.
CORPORATE SOURCE: Max-Planck-Inst. Kohlenforsch., Muelheim/Ruhr, Fed. Rep. Ger.
SOURCE: Justus Liebig's Annalen der Chemie (1969), 719, 169-86
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
AB RBX2 and R2BX (where (R = Me, Et, Pr, iso-Pr, Bu, Ph, cyclohexyl,

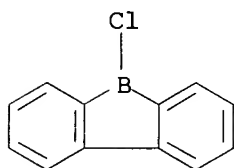
C₈H₁₇, C₁₀H₂₁, or PhCH₂; and X = Cl, F, Br, or I), were prepared by disproportionation of BX₃ with BR₃ in the presence of borohydrides. Yields were 75-99%. Borolanes, boraindane, borafluorenes and other boronated heterocycles were halogenated at the B atom by BX₃ (where X = Cl or Br). With BF₃, association compounds of the fluoroboronated heterocycle with BF₃ were obtained. RBI₂ were easily prepared from R₂BBR₂ and iodine.

IT 13059-59-1P 22072-86-2P

(preparation of)

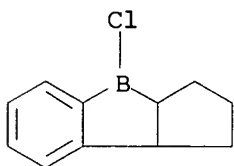
RN 13059-59-1 HCAPLUS

CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 22072-86-2 HCAPLUS

CN Benzo[b]cyclopenta[d]borole, 4-chloro-1,2,3,3a,4,8b-hexahydro- (8CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

IT 280-64-8P 367-45-3P 430-41-1P 589-69-5P 691-36-1P
 868-81-5P 1692-29-1P 1730-69-4P 1739-53-3P 3677-81-4P
 3857-03-2P 4151-77-3P 5158-50-9P 5314-83-0P 5674-70-4P
 13059-59-1P 13317-60-7P 13317-61-8P 14089-96-4P
 17933-10-7P 19162-10-8P 19162-11-9P 20905-32-2P
 21960-40-7P 21970-18-3P 21970-20-7P 21970-21-8P
 22072-73-7P 22072-74-8P 22072-75-9P 22072-76-0P,
 1H-1-Benzoborole, 1-[o-(2,3-dihydro-3-methyl-1H-1-benzoborol-1-yl)-
 β-methylphenethyl]-2,3-dihydro-3-methyl- 22072-77-1P
 22072-78-2P 22072-81-7P 22072-86-2P 22086-34-6P
 22086-35-7P 22086-36-8P 22086-37-9P 22086-40-4P
 22086-41-5P 22086-42-6P 22086-43-7P 22086-44-8P
 22086-45-9P 22086-46-0P 22086-47-1P 22086-51-7P
 22086-53-9P 22086-59-5P 22086-60-8P 22086-61-9P
 22086-63-1P 22086-64-2P 22086-65-3P 22137-00-4P
 22405-15-8P 23221-81-0P 23221-82-1P
 (preparation of)

L12 ANSWER 62 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

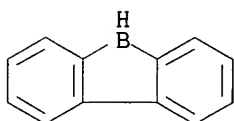
ACCESSION NUMBER: 1968:105310 HCAPLUS

DOCUMENT NUMBER: 68:105310

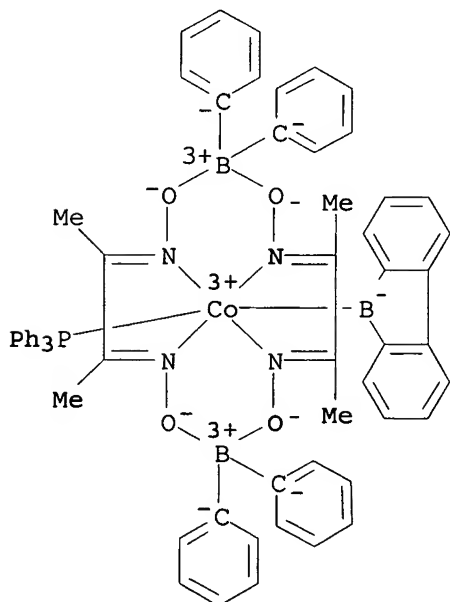
TITLE: Metal-boron compounds. VI.
 Bis(dimethylglyoximate)cobalt(III) compounds
 with cobalt-boron bonds

AUTHOR(S): Schmid, Guenter; Powell, Paul; Noeth, Heinrich

CORPORATE SOURCE: Univ. Marburg/Lahn, Marburg/Lahn, Fed. Rep. Ger.
 SOURCE: Chemische Berichte (1968), 101(4), 1205-14
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI For diagram(s), see printed CA Issue.
 AB The preps. of the complexes I (R = Ph, Bu) from bis(dimethylglyoximato)cobalt(III) chloride base adducts are described. These complexes react with metal carbonyl complexes to form $\text{Cl}_2\text{BMo}(\text{CO})_4(\text{PPh}_3)$, $\text{Cl}_2\text{BNi}(\text{NO})(\text{PPh}_3)_2$, $(\text{BF})\text{Mn}(\text{CO})_4(\text{PPh}_3)$ and $\text{Cl}_2\text{BFe}(\text{CO})_2(\text{C}_5\text{H}_5)$, where C_5H_5 is cyclopentadienyl.
 IT 244-33-7DP, 5H-Dibenzoborole, cobalt complexes
 18079-00-0P
 (preparation of)
 RN 244-33-7 HCAPLUS
 CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 18079-00-0 HCAPLUS
 CN Cobalt, [[bis[μ-[2,3-butanedione dioximato(2-)]]]tetraphenyldiborato(2-)]-5H-dibenzoborol-5-yl(triphenylphosphine)-, trans- (8CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)
 IT 244-33-7DP, 5H-Dibenzoborole, cobalt complexes
 431-03-8DP, 2,3-Butanedione, dioxime, cobalt complexes
 603-32-7DP, Arsine, triphenyl-, cobalt complexes 603-35-0DP,

Phosphine, triphenyl-, cobalt complexes 2386-98-3DP, Borane,
 bis(dimethylamino)-, cobalt complexes 10325-39-0DP, Borane,
 dichloro-, complexes with cobalt and iron and nickel 12306-68-2P
 13383-33-0DP, Borane, diphenyl-, cobalt complexes 14126-40-0P
 18078-93-8P 18078-99-4P **18079-00-0P** 18079-01-1P
 18079-02-2P 18115-35-0P 18115-36-1P 18115-37-2P
 18115-38-3P 18115-39-4P 18115-40-7P 18115-41-8P
 18115-42-9P 18115-43-0P 18115-45-2P 18115-46-3P
 18115-47-4P
 (preparation of)

L12 ANSWER 63 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:496377 HCAPLUS

DOCUMENT NUMBER: 67:96377

TITLE: Metal-boron compounds. V. Diarylboron group
 as a ligand in phosphine cobalt(II) compounds
 AUTHOR(S): Schmid, Guenter; Noeth, Heinrich
 CORPORATE SOURCE: Univ. Marburg/Lahn, Marburg/Lahn, Fed. Rep.
 Ger.

SOURCE: Chemische Berichte (1967), 100(9), 2899-907
 CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

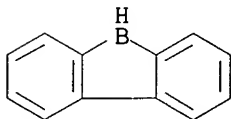
LANGUAGE: German

AB cf. CA 66: 28819k. R'₂CoH [where R' = (Ph₂PCH₂)₂ or
 o-C₆H₄(PMe₂)₂] were treated with R₂BCl (where R₂B = Ph₂B or
 9-borafuorenyl) to form R'₂CoCl₂ and trans-R'₂CO(BR₂)₂ and H₂.
 The R₂B group carried a neg. charge, and could be exchanged by
 ligand exchange reaction, as shown by the formation of compds.
 with Fe-B, Mn-B, Ni-B, Au-B bonding.

IT **244-33-7DP**, 5H-Dibenzoborole, cobalt complexes
18154-62-6P
 (preparation of)

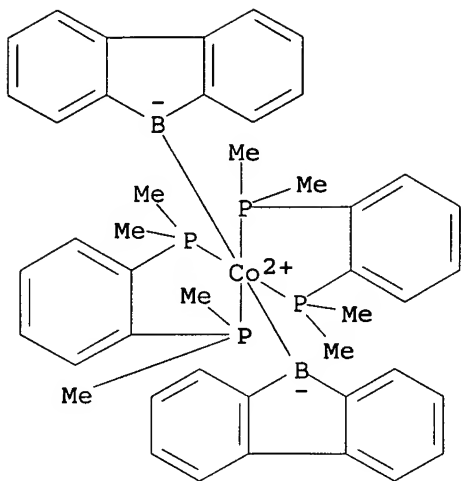
RN 244-33-7 HCAPLUS

CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 18154-62-6 HCAPLUS

CN Cobalt, bis(5H-dibenzoborol-5-yl)bis[o-
 phenylenebis(dimethylphosphine)]-, trans- (8CI) (CA INDEX NAME)



CC 78 (Inorganic Chemicals and Reactions)

IT 244-33-7DP, 5H-Dibenzoborole, cobalt complexes
 603-35-0DP, Phosphine, triphenyl-, gold complex 1663-45-2DP,
 Phosphine, ethylenebis[diphenyl-, complexes with cobalt and nickel
 4426-21-5P 5123-17-1P 7237-07-2DP, Phosphine,
 o-phenylenebis(dimethyl-, cobalt complexes 12277-78-0P
 13383-33-0DP, Borane, diphenyl-, transition metal complexes
 15555-90-5P 16985-95-8P 16985-96-9P 16997-64-1P
 17000-09-8P 18154-61-5P 18154-62-6P 18194-97-3P
 18194-98-4P 18347-83-6P 18556-96-2P 19293-29-9P
 19293-30-2P
 (preparation of)

L12 ANSWER 64 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:115757 HCAPLUS

DOCUMENT NUMBER: 66:115757

TITLE: Boron compounds. XI. Pyrolysis products of
 aralkyl and arylboranes

AUTHOR(S): Koester, Roland; Benedikt, Gerald; Fenzl,
 Wolfgang; Reinert, Klaus

CORPORATE SOURCE: Max-Planck-Inst. Kohlenforschung,
 Muelheim-Ruhr, Fed. Rep. Ger.

SOURCE: Justus Liebig's Annalen der Chemie (1967), 702,
 197-23

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: German

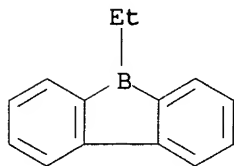
GI For diagram(s), see printed CA Issue.

AB cf. CA 64, 6688h. Aralkylboranes and arylcycloalkylboranes are
 converted on heating into B-containing heterocyclic compds.
 (1-boraindanes, 1-boratetralins, tricyclic boranes) with
 B-Caryl-bond. In contrast to the pyrolysis of trialkylboranes,
 not only does the reaction of a BH group with a sterically
 favorable Caryl-H formed by dehydroboration (cleavage of alkene)
 play a role, but also does the direct cleavage of aralkane,
 arylcycloalkane, or alkane. The ring closure of
 2-biphenyllylboranes to 9-borafluorenes (I) is also described.

IT 14855-16-4P
 (preparation and v and uv spectra of)

RN 14855-16-4 HCAPLUS

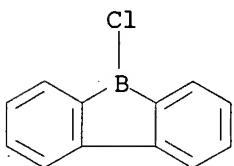
CN 5H-Dibenzoborole, 5-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 13059-59-1P 14010-92-5P 14010-93-6P
14010-95-8P 14265-95-3P 14265-96-4P
14855-11-9P, Benzo[b]cyclopenta[d]borole,
1,2,3,3a,4,8b-hexahydro-4-propyl- 14855-12-0P
(preparation of)

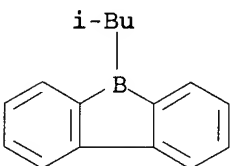
RN 13059-59-1 HCAPLUS

CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



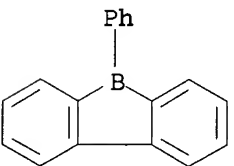
RN 14010-92-5 HCAPLUS

CN 5H-Dibenzoborole, 5-isobutyl- (7CI, 8CI) (CA INDEX NAME)



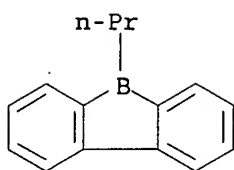
RN 14010-93-6 HCAPLUS

CN 5H-Dibenzoborole, 5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

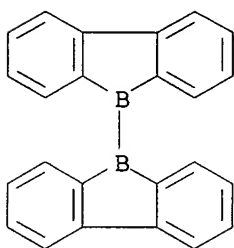


RN 14010-95-8 HCAPLUS

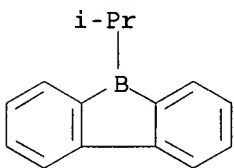
CN 5H-Dibenzoborole, 5-propyl- (7CI, 8CI) (CA INDEX NAME)



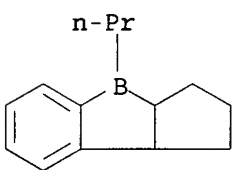
RN 14265-95-3 HCAPLUS
CN 5,5'-Bi-5H-dibenzoborole (8CI, 9CI) (CA INDEX NAME)



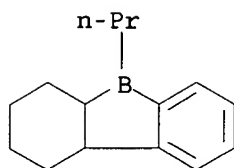
RN 14265-96-4 HCAPLUS
CN 5H-Dibenzoborole, 5-isopropyl- (7CI, 8CI) (CA INDEX NAME)



RN 14855-11-9 HCAPLUS
CN Benzo[b]cyclopenta[d]borole, 1,2,3,3a,4,8b-hexahydro-4-propyl- (8CI) (CA INDEX NAME)



RN 14855-12-0 HCAPLUS
CN 5H-Dibenzoborole, 1,2,3,4,4a,9b-hexahydro-5-propyl- (8CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

IT 14855-16-4P

(preparation and v and uv spectra of)

IT 13059-59-1P 13213-09-7P 14010-82-3P 14010-83-4P

14010-84-5P 14010-85-6P 14010-86-7P 14010-87-8P

14010-88-9P 14010-89-0P 14010-90-3P 14010-91-4P

14010-92-5P 14010-93-6P 14010-95-8P

14108-05-5P 14108-06-6P 14108-07-7P 14108-08-8P

14108-09-9P 14108-10-2P 14265-95-3P

14265-96-4P 14855-08-4P 14855-09-5P 14855-10-8P

14855-11-9P, Benzo[b]cyclopenta[d]borole,

1,2,3,3a,4,8b-hexahydro-4-propyl- 14855-12-0P

14855-13-1P 14855-14-2P, Dibenzo[b,e]borin, 1,2,3,4,4a,5,10,10a-

octahydro-5-propyl- 14855-15-3P, Naphtho[1,8-bc]borole,

1-ethyl-1,2-dihydro-

(preparation of)

L12 ANSWER 65 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1966:465472 HCAPLUS

DOCUMENT NUMBER: 65:65472

ORIGINAL REFERENCE NO.: 65:12186a-h,12187a-f

TITLE: Derivatives of methylenedioxybenzene. XX.

3,4:3',4'-Bis- [methylenedioxy]biphenyl

AUTHOR(S): Dallacker, Franz; Adolphen, Gerd

CORPORATE SOURCE: Tech. Hochsch., Aachen, Germany

SOURCE: Justus Liebigs Annalen der Chemie (1966), 694, 110-16

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: German

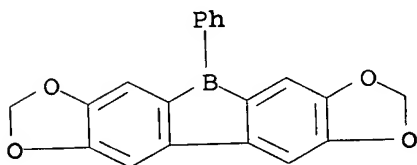
GI For diagram(s), see printed CA Issue.

AB cf. CA 65, 12153g. The preparation and substitution reactions of the title compound (I) are described. The ir spectra of the compds. were in accord with the structures reported. Cu bronze (120 g.) and 66 g. 3,4-CH₂O₂C₆H₃I (II) heated 2-3 hrs. at 200° in an oil bath, the mixture extracted (Soxhlet) 5 hrs. with Me₂CO, the extract concentrated, the residue distilled in vacuo, and the fraction b₄ 187-92°, crystallized from C₆H₆ gave 6.8 g. I, m. 145-6°. (I, R, =, R₁, =, H); (IV, R, =, R₁, =, NO₂); (V, R, =, Br, R₁, =, H); (VI, R, =, CO₂H, R₁, =, H); (VIII, R, =, CO₂Me, R₁, =, H); (IX, R, =, NO₂, R₁, =, H); (X, R, Br, R₁, =, NO₂); (XI, R, =, R₁, =, Br); (XII, R, =, R₁, =, I); (XIII, R, =, R₁, =, CO₂H); (XIV, R, =, R₁, =, CH₂Cl); (XV, R, =, R₁, =, CH₂OMe); (XVII, R, =, R₁, =, NH₂); To 30 g. II and 210 cc. Ac₂O was added portionwise 45 g. Cu(NO₃)₂·6H₂O with stirring at below 65° and the mixture stirred 1 hr. at room temperature and poured onto ice to give 29.3 g. 6-NO₂ derivative (III) of II, m. 109-10° (EtOH). II (20 g.) added dropwise to 150 cc. HNO₃ (d. 1.41) with stirring and the mixture stirred 30 min. and poured onto ice gave 22.4 g. III. III (30 g.) in 150 cc. PhNO₂ treated portionwise with 20 g. Cu bronze with stirring at 160° in such a way that only a slight

temperature rise occurred, the mixture stirred 30 min. and cooled, the precipitate filtered off and washed with Me₂CO, and the combined filtrate and washings concentrated in vacuo gave 11.2 g. IV, m. 225-6° (EtOH). A similar larger scale reaction of 120 g. III in 360 cc. PhNO₂ with 100 g. Cu bronze gave 64 g. IV. To 10 g. I in 150 cc. AcOH was added dropwise 2.5 cc. Br in 7 cc. AcOH at 60-70° and the solution stirred 30 min. and poured onto ice to give 9.5 g. V, m. 106° (EtOH). To BuLi solution (from 0.5 g. Li, 7.5 g. BuBr, and 150 cc. absolute Et₂O) was added 5 g. V at -15° under anhydrous conditions (N atmospheric), after 20 min. solid CO₂ added, the solution decomposed with H₂O, the layers separated, the Et₂O layer washed with H₂O, the combined aqueous solns. acidified with dilute HCl, and the precipitate filtered off and purified by repptn. from 2N NaOH with 2N HCl to give 2.5 g. VI, decomposed at 242-5°; evaporation of the Et₂O phase gave 1.4 g. VII. VI with Et₂O-CH₂N₂ gave VIII, m. 110-11° (EtOH). To 10 g. I in 500 cc. AcOH was added dropwise a mixture of 25 cc. 65% HNO₃ and 25 cc. AcOH at 10° with stirring, the mixture treated with an addnl. 50 cc. 65% HNO₃, and the precipitate filtered off to give 4.3 g. IX, m. 164-5° (EtOH); the filtrate poured into iced H₂O and the precipitate recrystd. from EtOH gave 3.7 g. IV. V (2 g.) in 150 cc. AcOH added dropwise during 30 min. to 50 cc. AcOH + 50 cc. 65% HNO₃ with stirring and the mixture stirred 30 min. and poured onto ice gave 1.2 g. X, m. 168-9° (EtOH). To 40 g. I in 250 cc. AcOH was added dropwise during 45 min. 20 cc. Br at 60-70° and after 1 hr. the solution poured onto ice to give 57.5 g. XI, m. 153-4° (EtOH). XI (4 g.) in 200 cc. absolute Et₂O treated with 1.3 g. BuLi in 45 cc. Et₂O with stirring under anhydrous conditions (N atmospheric), the solution kept 1 hr. at 0°, treated dropwise with 7.6 g. iodine in 50 cc. Et₂O, let stand 1 hr., and decomposed with ice, and the Et₂O layer separated, washed with aqueous NaHSO₃ and H₂O, dried, and evaporated gave 0.8 g. XII, m. 196-7° (EtOH). To BuLi solution (from 1 g. Li, 15 g. BuBr, and 150 cc. Et₂O) was added during 45 min. 8 g. XI in 500 cc. Et₂O under anhydrous conditions (N atmospheric), after 1 hr. solid CO₂ added, the solution decomposed with H₂O, and the aqueous layer separated and acidified with dilute HCl. to give 1.4 g. XIII, m. 293-4° (EtOH) [di-Me ester (via Et₂O-CH₂N₂) m. 158° (EtOH)]; from the Et₂O phase was isolated 3.7 g. VII, m. 279° (AcOH). Into a mixture of 40 g. I, 360 cc. AcOH, 500 cc. 12N HCl, and 40 g. paraformaldehyde was introduced a vigorous stream of HCl 2 hrs. at 90-100°, the mixture cooled and poured onto ice, and the solid filtered off, washed neutral with H₂O, and recrystd. repeatedly from cyclohexane to give 17.3 g. XIV, not anal. pure, decomposed at 248-51°. XIV (2 g.) refluxed 4-5 hrs. with a solution of 0.5 g. Na in 20 cc. MeOH, the solution poured into H₂O, the precipitate dissolved in boiling EtOH, and the solution treated with C, filtered, and diluted with H₂O gave 1.9 g. XV, m. 112°. A mixture of 2 g. XIV, 30 cc. H₂O, 5 g. KOH, and 5 cc. Me₂CO refluxed 16 hrs. and cooled, the precipitate filtered off, washed with H₂O, and dissolved in hot EtOH, and the solution diluted with H₂O gave 1.7 g. XVI, decomposed at 214-16°. A mixture of 12.1 g. I, 12 g. paraformaldehyde, 120 cc. 65% HBr, and 500 cc. AcOH stirred under ice cooling, heated gradually to 40° and finally 1 hr. at 45°, and poured onto ice gave 13.1 g. XVI. IV (25 g.) in 21. EtOH hydrogenated over Raney Ni 7 hrs. at 70°, the solution filtered and evaporated, the residue extracted repeatedly with dilute HCl, and the combined exts. made alkaline gave 2 g. XVII. IV (30 g.) in 11. AcOH heated to boiling with stirring, Raney Ni added, H introduced 10 hrs. at the b.p., the solution cooled, filtered, and diluted with H₂O, and the precipitate purified as

above gave 20 g. XVII, decomposed at 214-15°. XVII (2.7 g.) diazotized and the diazonium solution added to excess aqueous K2S with stirring and ice cooling, heated 45 min. at 100°, and cooled gave 2.2 g. XVIII, decomposed at 270-5° (EtOH). A mixture of 10 g. 6-bromopiperonylic acid (CA 55, 3593e), 10 g. NaOPh, 30 g. PhOH, and 2 g. Cu bronze stirred 4 hrs. at 100°, the solidified mass steam distilled (to remove PhOH) and dissolved in Me2CO, and the solution filtered and evaporated gave 6.5 g. 2,4,5-HO2C(CH2O2)C6H2OPh (XIX), m. 172° Me ester (via Et2O-CH2N2) m. 83-4° (EtOH). XIX (2 g.) dissolved in 50 cc. AcCl by gentle heating and the solution cooled, treated with 1 cc. concentrated H2SO4, and let stand 1 hr. at room temperature gave 1.55 g. XX, m. 221-2° (EtOH). To BuLi solution (from 0.6 g. Li, 6 g. BuBr, and 100 cc. Et2O) was added a suspension of 8 g. XI in 100 cc. Et2O under anhydrous conditions (N atmospheric), followed after 15 min. by 4.8 g. PhB(Obu)2 in 50 cc. Et2O + 100 cc. absolute C6H6, the solution distilled through a Vigreux column until the boiling range reached 55-60°, heated 30 min. at 55-60°, and decomposed with H2O, and the aqueous layer separated and acidified to give 1.9 g. XXI, m. 115-17° (EtOH). XI (8 g.) in Et2O-C5H6 converted similarly to the di-Li derivative with BuLi solution (from 0.6 g. Li and 6 g. BuBr in Et2O), the solution treated with 2.55 g. Me2SiCl2, distilled as above to a b.p. of 60°, heated 3 hrs. at 60°, and decomposed with H2O, the organic phase separated and evaporated, and the oily residue triturated with Me2CO gave 1.8 g. XXII, m. 232-3° (EtOH). (XXI, X, =, BPh); (XXII, X, =, SiMe2); (XXIV, X, =, PPh); (XXV, X, =, AsPh); (XXVI, X, =, SbPh); (XXVII, X, =, PbPh2). Similar treatment of 1.7 g. BuLi, 4 g. XI, and 2.6 g. Ph2SiCl2 in Et2O-C6H6 gave after heating 1.5 hrs. at 60° followed by hydrolysis an insol. residue, which filtered off and digested with hot Me2CO gave 1.4 g. XXIII, decomposed at 340°. From 1.7 g. BuLi, 4 g. XI, and 1.8 g. PhPCl2 in Et2O-C6H6 was prepared like XXII 1.6 g. XXIV, m. 204-5° (EtOH). From 1.7 g. BuLi, 4 g. XI, and 2.3 g. PhAsCl2 in Et2O-C6H6 was similarly prepared 2 g. XXV, m. 231-2° (EtOH). From 0.64 g. BuLi, 2 g. XI, and 2.3 g. PhSbCl2 in Et2O-C6H6 was similarly prepared 1 g. XXVI, m. 242-4° (EtOH). From 1.3 g. BuLi, 4 g. XI, and 4.3 g. Ph2PbCl2 in Et2O-C6H6 was similarly prepared 2.9 g. XXVII, decomposed at 301-2° (C6H6).

IT 7235-54-3, 5H-Borolo[2,3-f:4,5-f']bis[1,3]benzodioxole,
5-phenyl-
(preparation of)
RN 7235-54-3 HCAPLUS
CN 5H-Borolo[2,3-f:4,5-f']bis[1,3]benzodioxole, 5-phenyl- (7CI, 8CI)
(CA INDEX NAME)



CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 4791-89-3, Biphenyl, 3,4:3',4'-bis(methylenedioxy) - 4791-90-6,
Biphenyl, 2,2'-dibromo-4,5:4',5'-bis(methylenedioxy) - 6707-94-4,
Diphenic acid, 4,5:4',5'-bis(methylenedioxy) - 6720-25-8,
10H-1,3-Dioxolo[4,5-b]xanthen-10-one 7106-74-3, Benzene,

1-iodo-4,5-(methylenedioxy)-2-nitro- 7106-75-4, Biphenyl,
 4,5:4',5'-bis(methylenedioxy)-2,2'-dinitro- 7106-76-5, Biphenyl,
 2-bromo-3',4':4,5-bis(methylenedioxy)- 7106-77-6,
 10H-Fluoreno[2,3-d:6,7-d']bis[1,3]dioxol-10-one 7106-78-7,
 2-Biphenylcarboxylic acid, 3',4':4,5-bis(methylenedioxy)-, methyl
 ester 7106-79-8, Biphenyl, 3',4':4,5-bis(methylenedioxy)-2-nitro-
 7106-80-1, Biphenyl, 2-bromo-4,5:4',5'-bis(methylenedioxy)-2'-
 nitro- 7106-82-3, Biphenyl, 2,2'-diiodo-4,5:4',5'-
 bis(methylenedioxy)- 7106-83-4, Biphenyl, 2,2'-bis(chloromethyl)-
 4,5:4',5'-bis(methylenedioxy)- 7106-84-5, Biphenyl,
 2,2'-bis(methoxymethyl)-4,5:4',5'-bis(methylenedioxy)-
 7106-85-6, Oxepino[3,4-f:5,6-f']bis[1,3]benzodioxole, 5,7-dihydro-
 7106-86-7, 2,2'-Biphenyldiamine, 4,5:4',5'-bis(methylenedioxy)-
 7106-87-8, 5H-Bis[1,3]dioxolo[4,5-b:4',5'-h]carbazole 7106-88-9,
 Benzoic acid, 4,5-(methylenedioxy)-2-phenoxy- 7106-89-0, Benzoic
 acid, 4,5-(methylenedioxy)-2-phenoxy-, methyl ester 7106-91-4,
 5H-Silolo[2,3-f:4,5-f']bis[1,3]benzodioxole, 5,5-dimethyl-
 7106-92-5, 5H-Silolo[2,3-f:4,5-f']bis[1,3]benzodioxole,
 5,5-diphenyl- 7106-93-6, 5H-Phospholo[2,3-f:4,5-
 f']bis[1,3]benzodioxole, 5-phenyl- 7106-95-8,
 5H-Plumbolo[2,3-f:4,5-f']bis[1,3]benzodioxole, 5,5-diphenyl-
 7159-30-0, 2-Biphenylcarboxylic acid, 3',4':4,5-
 bis(methylenedioxy)- 7235-54-3, 5H-Borolo[2,3-f:4,5-
 f']bis[1,3]benzodioxole, 5-phenyl- 15039-98-2,
 5H-Stibolo[2,3-f:4,5-f']bis[1,3]benzodioxole, 5-phenyl-
 (preparation of)

L12 ANSWER 66 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1966:443972 HCAPLUS

DOCUMENT NUMBER: 65:43972

ORIGINAL REFERENCE NO.: 65:8204c-d

TITLE: The electronic structure of the diphenylboron
 cation and the 9-borafluorenes

AUTHOR(S): Armstrong, D. R.; Perkins, P. G.

CORPORATE SOURCE: Univ. Newcastle-upon-Tyne, UK

SOURCE: Journal of the Chemical Society [Section] A:
 Inorganic, Physical, Theoretical (1966), (8),
 1026-31

CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal

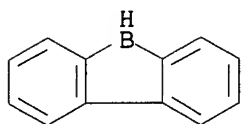
LANGUAGE: English

AB The electronic structures and absorption spectra of the
 diphenylboron and the 9-borafluorene cations, neutral
 borafluorene, and β -chloro-9-bora-fluorene are calculated by the
 Pariser-Parr-Pople technique. A comparison of the calculated with the
 observed energies indicates that in solution the Ph_2B^+ ion is
 coordinated while the 9-borafluorene cation is not. Similar
 considerations infer the highly polar nature of the B-R bond in
 the neutral 9-borafluorenes.

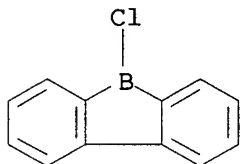
IT 244-33-7, 5H-Dibenzoborole 13059-59-1,
 5H-Dibenzoborole, 5-chloro-
 (cation from, electronic structure and spectrum of)

RN 244-33-7 HCAPLUS

CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 13059-59-1 HCAPLUS
 CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 10 (Spectra and Some Other Optical Properties)
 IT 244-33-7, 5H-Dibenzoborole 13059-59-1,
 5H-Dibenzoborole, 5-chloro- 13383-33-0, Borane, diphenyl-
 (cation from, electronic structure and spectrum of)

L12 ANSWER 67 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1966:427003 HCAPLUS
 DOCUMENT NUMBER: 65:27003
 ORIGINAL REFERENCE NO.: 65:4985g-h,4986a-b
 TITLE: Metal-boron compounds. III.
 Triphenylphosphinetetracarbonylmanganese-boron
 compounds
 AUTHOR(S): Noeth, H.; Schmid, G.
 CORPORATE SOURCE: Univ. Munich, Germany
 SOURCE: Zeitschrift fuer Anorganische und Allgemeine
 Chemie (1966), 345(1-2), 69-78
 CODEN: ZAACAB; ISSN: 0044-2313

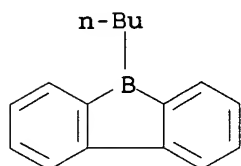
DOCUMENT TYPE: Journal
 LANGUAGE: German

GI For diagram(s), see printed CA Issue.

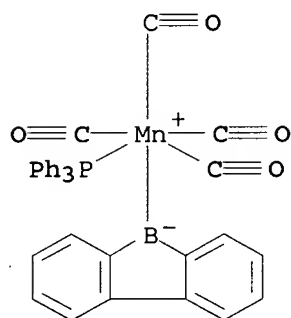
AB cf. CA 64, 6682c. The reaction of Ph_2BCl and $\text{NaMn}(\text{CO})_4\text{PPh}_3$ (I) in Et_2O in the presence of a small amount of Na amalgam gave a 60-70% yield of $\text{Ph}_2\text{BMn}(\text{CO})_4\text{PPh}_3$, m. 120° , which was recovered by filtration, removal of solvent, and recrystn. from petr. ether. $\text{Bu}_2\text{BMn}(\text{CO})_4\text{PPh}_3$ and a derivative of 9-borafluorene (II), m. $>140^\circ$, were prepared in similar fashion in yields of 33% and 52%, resp. $\text{Et}_2\text{PB}(\text{NEt}_2)_2\text{Cl}$ reacted with $\text{Ni}(\text{CO})_4$ at 0° to form $(\text{CO})_3\text{NiP}(\text{Et})_2\text{B}(\text{NEt}_2)_2\text{Cl}$ (III). III is a liquid which, in turn, reacted with I in Et_2O to give a 62% yield of $(\text{CO})_3\text{NiP}(\text{Et})_2\text{B}(\text{NEt}_2)\text{Mn}(\text{CO})_4\text{PPh}_3$. $\text{Cl}_2\text{BMn}(\text{CO})_4\text{PPh}_3$ (IV) was prepared in 60% yield by a reaction between BCl_3 and I in Et_2O . Extended reaction time causes IV to combine with more I to give a 66% yield of $\text{ClB}[\text{Mn}(\text{CO})_4\text{PPh}_3]_2$, m. 110° (decomposition). A similar reaction between I and Et_2NBCl_2 gave an 85% yield of $\text{Et}_2\text{NB}[\text{Mn}(\text{CO})_4\text{PPh}_3]_2$, m. 120° (decomposition). Reaction of IV with NaOMe in Et_2O gave a 76% yield of $(\text{MeO})_2\text{BMn}(\text{CO})_4\text{PPh}_3$. Reaction of IV with Me_2NH in Et_2O gave $\text{Me}_2\text{N}(\text{Cl})\text{BMn}(\text{CO})_4\text{PPh}_3$, m. $135-40^\circ$. A similar reaction with o-phenylenediamine gave a 77% yield of V, m. $120-25^\circ$. All of the B-Mn compds. are very sensitive to H_2O and O and all manipulations were carried out

under dry N. Br₂ or Ag⁺ will cleave the B-Mn bound. The compds. are all monomers in C₆H₆. Some ir and N.M.R. data are presented and discussed in terms of B-Mn π -bonding.

IT 7760-71-6, 5H-Dibenzoborole, 5-butyl- 15696-95-4
, 5H-Dibenzoborole, manganese complex
(preparation of)
RN 7760-71-6 HCAPLUS
CN 5H-Dibenzoborole, 5-butyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



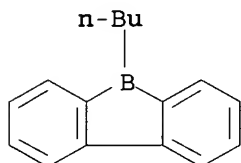
RN 15696-95-4 HCAPLUS
CN Manganese, tetracarbonyl-5H-dibenzoborol-5-yl(triphenylphosphine) -
(9CI) (CA INDEX NAME)



CC 14 (Inorganic Chemicals and Reactions)
IT 272-92-4, 2H-1,3,2-Benzodiazaborole, manganese complex
2052-07-5, Biphenyl, 2-bromo- 4542-61-4, Borane, dimethoxy-,
manganese complex 7760-71-6, 5H-Dibenzoborole, 5-butyl-
15660-49-8, Manganese, tetracarbonyl(dibutylboryl)(triphenylphosphine)-
15667-02-4, Manganese, (dichloroboryl)tetracarbonyl(triphenylphosphine)-
15679-57-9, Manganese, tetracarbonyl(diphenylboryl)(triphenylphosphine)-
15679-58-0, Manganese, (chloroborylene)bis[tetracarbonyl(triphenylphosphine)]-
15679-59-1, Manganese, [(diethylamino)borylene]bis[tetracarbonyl(triphenylphosphine)]-
15696-95-4, 5H-Dibenzoborole, manganese complex 15710-24-4, Manganese,
(dimethoxyboryl)tetracarbonyl(triphenylphosphine)- 15710-33-5, Manganese,
[chloro(dimethylamino)boryl]tetracarbonyl(triphenylphosphine)-
15752-06-4, Manganese, (2H-1,3,2-benzodiazaborolato)tetracarbonyl(triphenylphosphine)-
15818-83-4, Manganese, [μ -(diethylamino)(diethylphosphino)boryl]
(tricarbonylnickel)tetracarbonyl(triphenylphosphine)-
18494-92-3, Borane, (diethylamino)-, manganese complex
(preparation of)

L12 ANSWER 68 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1966:427002 HCAPLUS
DOCUMENT NUMBER: 65:27002

ORIGINAL REFERENCE NO.: 65:4985f-g
 TITLE: Dibromotetrakis(thiourea)manganese(II) complex
 AUTHOR(S): Dash, K. C.; Rao, D. V. Ramana
 CORPORATE SOURCE: Regional Eng. Coll., Rourkela, India
 SOURCE: Current Science (1966), 35(8), 203-4
 CODEN: CUSCAM; ISSN: 0011-3891
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB MnBr₂ and thiourea (1:4) were refluxed in EtOH for 2 hrs. The solution was concentrated and cooled to obtain white crystalline Mn[SC(NH₂)₂]Br₂, m. 179°. It is a nonelectrolyte in Me₂CO and has 5 unpaired electrons ($\mu = 6.03$ Bohr magnetons). Attempts to prepare the analogous iodide and thiocyanate complexes failed.
 IT 7760-71-6, 5H-Dibenzoborole, 5-butyl- (preparation of)
 RN 7760-71-6 HCAPLUS
 CN 5H-Dibenzoborole, 5-butyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 14 (Inorganic Chemicals and Reactions)
 IT 603-35-0, Phosphine, triphenyl- 2052-07-5, Biphenyl, 2-bromo-7760-71-6, 5H-Dibenzoborole, 5-butyl- 15660-49-8, Borane, dibutyl-, manganese complex 15679-57-9, Manganese, tetracarbonyl(diphenylboryl)(triphenylphosphine)- 16037-98-2, Manganese, dibromotetrakis(thiourea)- (preparation of)

L12 ANSWER 69 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

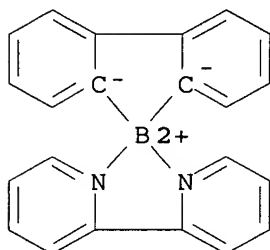
ACCESSION NUMBER: 1966:51908 HCAPLUS
 DOCUMENT NUMBER: 64:51908
 ORIGINAL REFERENCE NO.: 64:9679d-e
 TITLE: Some stable monoboron free radicals.
 2,2'-Bipyridine stabilization of unusual oxidation states of boron
 AUTHOR(S): Kuck, Mark A.; Urry, Grant
 CORPORATE SOURCE: Purdue Univ., Lafayette, IN
 SOURCE: Journal of the American Chemical Society (1966), 88(3), 426-31
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Treatment of various chloroboranes with lithium 2,2'-bipyridine, dilithium 2,2'-bipyridine, or with mixts. of these two reagents results in the formation of a series of neutral-monoboron compds. in which boron is stabilized in unusual oxidation states by chelation with 2,2'-bipyridine. Dimethylaminoboron 2,2'-bipyridine is an even-electron diamagnetic species while 2,2'-biphenyleneboron 2,2'-bipyridine, bis(dimethylamino)boron 2,2'-bipyridine, and boron bis(2,2'-bipyridine) all are odd-electron paramagnetic species. The characterizations of these compds. are discussed along with some of their chemical properties and E.S.R. spectra of

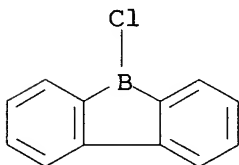
the paramagnetic species.

IT 15225-19-1, Boron, (2,2'-biphenylene) (2,2'-bipyridine) -
(preparation of)
RN 15225-19-1 HCAPLUS
CN Boron, [1,1'-biphenyl]-2,2'-diyl(2,2'-bipyridine-N,N')-, (T-4) -
(9CI) (CA INDEX NAME)



CC 37 (Heterocyclic Compounds (One Hetero Atom))
IT 536-75-4, Pyridine, 4-ethyl- 15225-19-1, Boron,
(2,2'-biphenylene) (2,2'-bipyridine) -
(preparation of)

L12 ANSWER 70 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1964:16940 HCAPLUS
DOCUMENT NUMBER: 60:16940
ORIGINAL REFERENCE NO.: 60:2997e-h
TITLE: Polynuclear complexes of ethyl(ethoxy)aluminum
chloride
AUTHOR(S): Scherer, H.; Seydel, G.
CORPORATE SOURCE: Farbwerke Hoechst A.-G., Frankfurt; Germany
SOURCE: Angew. Chem. (1963), 75(18), 846-51
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Infrared, reaction rate, and d. measurements on the system
EtOH:2Et2AlCl in C7H16 indicate the formation and isomerization of
Et(EtO)AlCl as follows:
IT 13059-59-1, 5H-Dibenzoborole, 5-chloro-
(preparation of)
RN 13059-59-1 HCAPLUS
CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)
IT 122-56-5, Borane, tributyl- 1107-40-0, Borane, tri-10-pinanyl-,
isomers 1116-61-6, Borane, tripropyl- 1123-02-0, Borolane,
1-butyl- 10325-42-5, Borane, diisopropylpropyl- 10325-43-6,
Borane, isopropylidipropyl- 13059-59-1, 5H-Dibenzoborole,
5-chloro- 13213-09-7, 1H-1-Benzoborole, 2,3-dihydro-1-phenethyl-
14010-85-6, 1H-1-Benzoborole, 2,3-dihydro-1-isobutyl-3-methyl-

14010-87-8, 1-Benzoborin, 1,2,3,4-tetrahydro-1-(3-phenylpropyl)-
 14108-09-9, 1H-1-Benzoborole, 1-butoxy-2,3-dihydro-3-methyl-
 16664-33-8, 9b-Boraphenalene, dodecahydro- 91636-09-8, Borane,
 dibutylisobutyl- 92658-67-8, Borepane, 1-ethyl- 92658-68-9,
 Borinane, 1-ethyl-2-methyl- 92672-98-5, Borolane, 1,2-diethyl-
 93113-81-6, 1,3,5,7-Tetraborocane, 1,3,5,7-tetramethyl-
 94981-88-1, Borinane, 1-isoheptyl-3-methyl- 94981-89-2, Borolane,
 1-isoheptyl-2,4-dimethyl- 98493-50-6, 1H-1-Benzoborole,
 1-(o-ethylphenyl)-2,3-dihydro- 878191-98-1, Borepane,
 1-ethyl-3,6-dimethyl-, trans- 878192-04-2, Borepane,
 1-ethyl-3,6-dimethyl-, cis- 878192-11-1, Borolane,
 1-ethyl-3,4-dimethyl-, trans- 878192-37-1, Borolane,
 1-ethyl-3,4-dimethyl-, cis-
 (preparation of)

L12 ANSWER 71 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1964:16939 HCAPLUS

DOCUMENT NUMBER: 60:16939

ORIGINAL REFERENCE NO.: 60:2997d-e

TITLE: Conversion of boron-organic compounds under heating

AUTHOR(S): Koester, R.; Benedikt, G.; Larbig, W.; Reinert, K.; Rotermund, G.

CORPORATE SOURCE: Max-Planck-Inst., Muelheim/Ruhr, Germany

SOURCE: Angew. Chem. (1963), 75(22), 1079-90

DOCUMENT TYPE: Journal

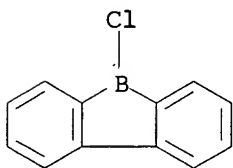
LANGUAGE: Unavailable

AB Trialkylboranes with the same or different radicals on the B-atom are stable to alkyl exchange at room temperature. However, trialkylboranes undergo disproportionation at higher temperature without catalyst. Gas-chromatographic analysis proved that Pr_3B gave 16% iso- PrBPr_2 and 1% (iso- Pr) $_2\text{BPr}$ at 160°, and Bu_3B gave 6% iso- BuBBu_2 at 160°. Examples of thermal isomerization and irreversible pyrolytic reactions are reviewed with 60 references.

IT 13059-59-1, 5H-Dibenzoborole, 5-chloro-
 (preparation of)

RN 13059-59-1 HCAPLUS

CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)

IT 122-56-5, Borane, tributyl- 1107-40-0, Borane,
 tris[(6,6-dimethylbicyclo[3.1.1]hept-2-yl)methyl]- 1116-61-6,
 Borane, tripropyl- 1123-02-0, Borolane, 1-butyl- 10325-42-5,
 Borane, diisopropylpropyl- 10325-43-6, Borane,
 isopropylidipropyl- 13059-59-1, 5H-Dibenzoborole,
 5-chloro- 13213-09-7, 1H-1-Benzoborole, 2,3-dihydro-1-phenethyl-
 14010-85-6, 1H-1-Benzoborole, 2,3-dihydro-1-isobutyl-3-methyl-
 14010-87-8, 1-Benzoborin, 1,2,3,4-tetrahydro-1-(3-phenylpropyl)-
 14108-09-9, 1H-1-Benzoborole, 1-butoxy-2,3-dihydro-3-methyl-
 16664-33-8, 9b-Boraphenalene, dodecahydro- 91636-09-8, Borane,
 dibutylisobutyl- 92672-98-5, Borolane, 1,2-diethyl-

93113-81-6, 1,3,5,7-Tetraborocane, 1,3,5,7-tetramethyl-
 94981-88-1, Borinane, 1-isoheptyl-3-methyl- 94981-89-2, Borolane,
 1-isoheptyl-2,4-dimethyl- 98493-50-6, 1H-1-Benzoborole,
 1-(o-ethylphenyl)-2,3-dihydro-
 (preparation of)

L12 ANSWER 72 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1963:441875 HCAPLUS

DOCUMENT NUMBER: 59:41875

ORIGINAL REFERENCE NO.: 59:7574b-h,7575a-e

TITLE: The chemical constituents of Australian
 Flindersiaspecies. XVII. The structure of
 ifflaiamine

AUTHOR(S): Bosson, Judith A.; Rasmussen, M.; Ritchie, E.;
 Robertson, A. V.; Taylor, W. C.

CORPORATE SOURCE: Univ. Sydney

SOURCE: Australian Journal of Chemistry (1963), 16(3),
 480-90

CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. CA 58, 14439e. A new alkaloid ifflaiamine (I) and a new
 triterpene acid (II) have been isolated from the wood of
 Flindersia ifflaiana F. Muell. The milled wood (13.3 kg.) was
 percolated successively with ligroine, ether, acetone and MeOH.
 Solvent was removed from the light petr. extract, residue dissolved
 in ether and separated into 5% HCl, 5% NaHCO₃, 2% Na₂CO₃, and 2% NaOH
 soluble and neutral fraction. The HCl extract on basification and extraction
 with CHCl₃ gave 1.9 g. crude I. The NaHCO₃-soluble fraction gave 4.3
 g. oil from which no crystalline substance could be isolated even after
 methylation with CH₂N₂ and chromatography on Al₂O₃. The Na₂CO₃
 extract gave 34 g. crude II while no phenolic substance was obtained
 from NaOH fraction. The neutral fraction gave 135 g. thick brown
 intractable oil. The ether extract similarly gave 6.9 g. crude I and
 the acetone extract, 2.1 g. crude I; no crystalline substance was obtained
 from the MeOH extract. For purification of II, 10.3 g. crude acid was
 methylated with CH₂N₂ in ether which on chromatography on Al₂O₃
 gave 7.7 g. Me ifflaionate, m. 175°, [α]_D²⁰
 59° (c 1.0, CHCl₃). Refluxing the ester with 10% alc. KOH
 for 3 hrs. gave pure II, m. 259-60°, [α]_D²⁰
 88° (c 1.0, CHCl₃). The crude alkaloid on repeated
 chromatography on Al₂O₃ gave I.H₂O, C₁₅H₁₇O₂N.H₂O, m.
 62-3°. Anhydrous I obtained by drying at 80°/1 mm. on
 P₂O₅ was a gum, [α]_D²⁵ 589 -0.6 and [α]_D²⁵ 420
 -3.6° (c 8.0, MeOH); picrate m. 207-9°. I was a
 weak base, formed no quaternary salts, had one methylimino group,
 a terminal Me group, and no OMe groups. It could not be
 hydrogenated at room temperature in HOAc or in presence of HClO₄ and Pt.
 The ultraviolet and infrared spectra showed it to be a
 2-alkoxy-4-quinolone, unlike all other alkaloids isolated from
 Flindersia spp. which are 4-alkoxy-2-quinolones. The ultraviolet
 spectrum in EtOH (neutral or alkaline) showed λ_{maximum} 215, 236,
 251 (shoulder), 298 (inflection), 309, 320 mμ, log ε
 4.51, 4.39, 4.18, 3.91, 4.05, and 4.01; λ_{min}. 265 mμ,
 log ε 3.30; in 0.2N acid solution there was a hypsochromic
 shift in long wavelength bands while intensities increased at both
 short and long wavelength regions: λ_{maximum} 216, 235, 294, 315
 (inflection) mμ, log ε 4.52, 4.59, 4.10, 3.83.
 However, in cyclohexane there was a bathochromic shift and

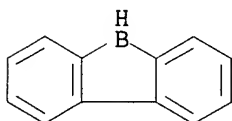
decrease in intensities: λ_{maximum} 236 (shoulder), 251, 261, 275, 288 (inflection), 305 (inflection), 315, 326 μ , $\log \epsilon$ 4.25, 4.10, 4.19, 3.52, 3.48, 3.81, 3.96, and 3.87. Infrared spectrum showed ν 1504, 1538, 1597, and 1623 cm^{-1} in Nujol and 1508, 1541, 1585, and 1617 cm^{-1} in CHCl_3 . Structure was suggested I for ifflaiamine. A solution of 1 g. I and 10 g. KOH in 100 ml. EtOH was refluxed for 30 hrs., diluted with 100 ml. H_2O , concentrated to 100 ml., and extracted with CHCl_3 to give 0.15 g. I. The aqueous solution was saturated with CO_2 and extracted with CHCl_3 to give 0.75

g.

of a phenol which was purified by sublimation at $180-90^\circ/0.3$ mm. and crystallization to give pure IV, m. $220-2^\circ$, λ (EtOH) 224, 241 (shoulder), 259 (shoulder), 290 (shoulder), 315 μ , $\log \epsilon$ 4.55, 4.40, 3.89, 3.74, 3.97; λ_{maximum} (in N NaOH in EtOH) 234, 241 (shoulder), 256 (shoulder), 265 (shoulder), 314 μ , $\log \epsilon$ 4.29, 4.23, 4.03, 3.78, 4.04; λ_{maximum} (in N HCl in EtOH) 232, 281, 289, 308 (shoulder), 318, 331 (shoulder) μ , $\log \epsilon$ 4.55, 3.83, 3.85, 3.70, 3.79, 3.64; ν_{maximum} 1513, 1585, 1613, 1642 cm^{-1} (Nujol). A solution of 0.3 g. IV in 30 ml. 6N HCl was refluxed for 24 hrs., diluted with 60 ml. H_2O , and extracted with CHCl_3 to give 0.2 g. gum, ν_{maximum} 1499, 1570, 1592, 1623, and 1657 cm^{-1} with weak bands in the region 1500-1600 cm^{-1} . The more basic aqueous fraction gave I. The spectral properties of the gum indicated the presence of V. Due to the unusual structure of I its synthesis was attempted. A mixture of 10.7 g. methylaniline and 48 g. malonic ester was refluxed so that EtOH formed escaped freely through the air condenser. After cooling, the mixture was diluted with petr. ether, filtered, the solid dissolved in 300 ml. 3% NaOH, the solution treated with charcoal and filtered, the filtrate acidified, and the solid separated. The solid was stirred with 200 ml. boiling EtOH, cooled and insol. material collected. The filtrate was evaporated to dryness, and the residue extracted with 300 ml. 3N HCl, and treated with NaOAc to give a precipitate of 2.6 g. 1-methyl-4-hydroxy-2-quinolone (VI), m. 267° . The sparingly soluble substance gave 5.5 g. VII, m. $255-6^\circ$, λ_{maximum} (EtOH) 242, 255, 270, 350, and 365 μ , $\log \epsilon$ 4.42, 4.29, 3.95, 3.73, 3.88, 3.91, 3.94, and 3.91. Under milder conditions, i.e. when a solution of 10.7 g. methylaniline and 17.6 g. malonic ester in 50 ml. Ph 2O was refluxed for 1 hr. and worked up as above it gave 1.7 g. VI and 7 g. VII. A mixt. of 1.7 g. VI and 10 g. malonic ester was refluxed 1.5 hrs. to give 1.9 g. VII. A solution of 3 g. VII in 20 ml. H_2O and 20 ml. H_2SO_4 on refluxing for 1 hr. gave a quant. yield of VI. A mixture of 9.39 g. aniline and 100 g. malonic ester was heated in an open flask. At 165° EtOH started evolving. The temperature was raised to 200° during 0.5 hr. and maintained for 0.5 hr. more. The unreacted ester was distilled as much as possible and residue diluted with 2 vols. benzene. The solution on keeping deposited 2.1 g. malonanilide, whereas the mother liquor gave half-ester anilide. The half-ester anilide (7 g.) was added to boiling 100 ml. Ph 2O , and after 5 min. diluted with petr. ether to give 3 g. malonanilide. The half-ester anilide (2 g.) was heated with 20 g. polyphosphoric acid at 170° for 0.5 hr. Worked up as for VI, the reaction mixture gave 1 g. 4-hydroxy-2-quinolone (VIII), m. $350-2^\circ$. As in the case of VI, refluxing a mixture of 0.3 g. VIII and 30 g. malonic ester for 1.7 hrs. gave IX, m. 315° . On boiling with H_2SO_4 IX gave VIII. Similar methods when applied to the synthesis of 3-acetonyl-4-hydroxy-2-quinolones gave only tars. Di-Me phenacylmalonate (X) (2.5 g.), b 1 164° , m. 76° , and 0.9 g. aniline in 10 ml. Ph 2O was

heated in an open flask at 210° for 0.5 hr. to give 0.2 g. phenacylmalonilide, m. 210°, and 0.7 g. Me phenacylmalonanilate, m. 125-6°. Heating 1.7 g. half ester anilide with 25 g. polyphosphoric acid at 140-50° for 10 min. gave 0.6 g. β -benzoylpropionanilide, m. 150°, the possible mechanism for the formation of which is discussed. It was also obtained by heating 0.2 g. aniline with 0.35 g. γ -phenylcrotonolactone at 180-90° for 10 min.

IT 244-33-7, 5H-Dibenzoborole
(preparation of)
RN 244-33-7 HCAPLUS
CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 41 (Alkaloids)
IT 86-95-3, Carbostyryl, 4-hydroxy- 244-33-7,
5H-Dibenzoborole 1677-46-9, Carbostyryl, 4-hydroxy-1-methyl-
6805-19-2, Ifflaionic acid 17649-94-4, Propionanilide,
3-benzoyl- 18706-63-3, 3-Quinolineacrylic acid,
1,2-dihydro- β ,4-dihydroxy-1-methyl-2-oxo-, δ -lactone
31520-89-5, Furo[3,2-c]quinolin-4(2H)-one, 3,5-dihydro-2,3,3,5-
tetramethyl- 31520-96-4, Ifflaiamine, picrate 93407-59-1,
2-Thiophenebutyramide, N-[3,4-(methylenedioxy)phenethyl]-
94091-83-5, Carbostyryl, 4-hydroxy-3-(2-hydroxy-1,1-
dimethylpropyl)-1-methyl- 94891-68-6, 3-Quinolineacrylic acid,
1,2-dihydro- β ,4-dihydroxy-2-oxo-, δ -lactone
95168-61-9, Malonanilic acid, 2-phenacyl-, methyl ester
100734-76-7, Malonanilide, 2-phenacyl-
(preparation of)

L12 ANSWER 73 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

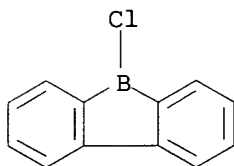
ACCESSION NUMBER: 1963:441771 HCAPLUS
DOCUMENT NUMBER: 59:41771
ORIGINAL REFERENCE NO.: 59:7547d-g
TITLE: 9-Borafluorenes
AUTHOR(S): Koester, R.; Benedikt, G.
CORPORATE SOURCE: Max-PlanckInst., Muelheim/Ruhr, Germany
SOURCE: Angew. Chem. (1963), 75, 419
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

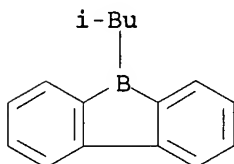
AB 2-Biphenylyldialkylboranes, preparable from 2-lithiobiphenyl (I) and dialkylchloroboranes, split out alkane at 180-200° to give a 9-alkyl-9-borafluorene (II). The following II were prepared [R, b.p./mm., m.p., % yield, ν (cm.⁻¹ given): Et, 112°/0.3, 16°, 65, 25,800; Pr and iso-Pr (mixture), 130°/0.2, 5°, 42, -, iso-Bu, 140°/0.2, 13.5°, 40, -; Ph (temperature of 280 300° required), 180°/0.4, 118°, 56, 24,700. All I were intensely yellow, which was attributable to a disturbance of the system by the B atom. From II (R = alkyl or aryl) and BCl₃ in the presence of BH compds. was prepared II (R = Cl), yellow, b_{0.1} 110°, m. 52°, ν 25,200 cm.⁻¹, along with RBCl₂ (R = alkyl or aryl). II formed colorless

etherates; the di-Et etherate dissociated on melting (82°). Treatment of Na+(BET₃H) and II (R = Cl) in hexane gave bis(9-borafluorene), colorless, ν 1545 cm.⁻¹, which dissociated on heating (80°) in C₆H₆ to give II (R = H), yellow, ν 2500 cm.⁻¹ 9-Alkyl- or 9-aryl-9-borafluorenes on treatment with AlEt₃ gave BET₃ and dimeric 9-alkyl or 9-aryl-9-aluminafluorenes. Pyrolysis of I and dialkyl- or diarylchloroboranes (mole ratio: 2:1) gave III.

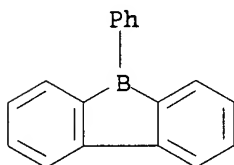
IT 13059-59-1, 5H-Dibenzoborole, 5-chloro- 14010-92-5
 , 5H-Dibenzoborole, 5-isobutyl- 14010-93-6,
 5H-Dibenzoborole, 5-phenyl- 14855-16-4,
 5H-Dibenzoborole, 5-ethyl- 89306-12-7, 5H-Dibenzoborole,
 dimer 108479-75-0, Lithium bis(2,2'-biphenylene)borate
 (preparation of)
 RN 13059-59-1 HCAPLUS
 CN 5H-Dibenzoborole, 5-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)



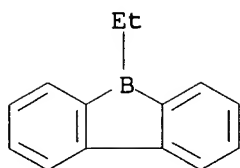
RN 14010-92-5 HCAPLUS
 CN 5H-Dibenzoborole, 5-isobutyl- (7CI, 8CI) (CA INDEX NAME)



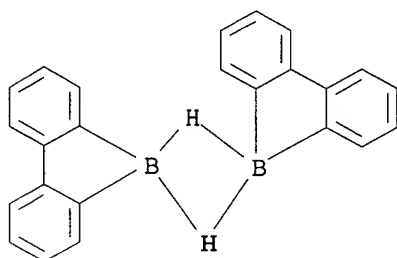
RN 14010-93-6 HCAPLUS
 CN 5H-Dibenzoborole, 5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



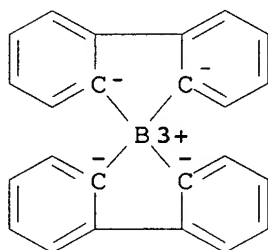
RN 14855-16-4 HCAPLUS
 CN 5H-Dibenzoborole, 5-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 89306-12-7 HCAPLUS
 CN 5H-Dibenzoborole, dimer (7CI) (CA INDEX NAME)



RN 108479-75-0 HCAPLUS
 CN Borate(1-), bis([1,1'-biphenyl]-2,2'-diyl)-, lithium, (T-4)- (9CI)
 (CA INDEX NAME)



● Li⁺

CC 39 (Organometallic and Organometalloidal Compounds)
 IT 13059-59-1, 5H-Dibenzoborole, 5-chloro- 14010-92-5
 , 5H-Dibenzoborole, 5-isobutyl- 14010-93-6,
 5H-Dibenzoborole, 5-phenyl- 14855-16-4,
 5H-Dibenzoborole, 5-ethyl- 35256-13-4, Titanium,
 ethoxybis(8-quinolinolato)cyclopentadienyl- 89306-12-7,
 5H-Dibenzoborole, dimer 108479-75-0, Lithium
 bis(2,2'-biphenylene)borate
 (preparation of)

L12 ANSWER 74 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1963:14974 HCAPLUS
 DOCUMENT NUMBER: 58:14974
 ORIGINAL REFERENCE NO.: 58:2469h,2470a
 TITLE: Synthesis of (bisbiphenylene)arylsoranes

from spirobisbiphenylene arsonium salts

AUTHOR(S): Wittig, G.; Hellwinkel, D.
 CORPORATE SOURCE: Univ. Heidelberg, Germany
 SOURCE: Angew. Chem. (1962), 74, 782
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

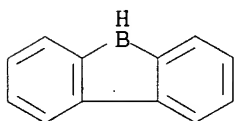
GI For diagram(s), see printed CA Issue.

AB Biphenylene-o-biphenylyldichloroarsorane (I) or bis-o-biphenylyltrichloroarsorane split off HCl at 250° to produce in good yield spiro(bisbiphenylene)arsonium chloride, m. 319°, with isomerization to biphenylene-2-(2'-chlorodiphenyl)arsine. Other salts prepared were the iodide, m. 309-11°, the tetraphenylborate, m. 257.5-9.5°, and the bisbiphenylene borate, m. 290-1°. Reaction of these salts with PhLi or p-Me₂NC₆H₄Li produced bisbiphenylenearylsoranes in good yield.

IT 244-33-7, 5H-Dibenzoborole (spiro derivative)

RN 244-33-7 HCAPLUS

CN 5H-Dibenzoborole (7CI, 8CI, 9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)

IT 244-33-7, 5H-Dibenzoborole (spiro derivative)

L12 ANSWER 75 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

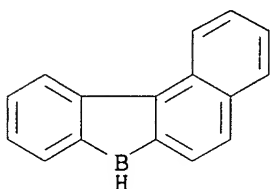
ACCESSION NUMBER: 1962:416985 HCAPLUS
 DOCUMENT NUMBER: 57:16985
 ORIGINAL REFERENCE NO.: 57:3464e-h
 TITLE: Optically active organic boron compounds. IV. Preparation of a quadrivalent borospiro
 AUTHOR(S): Torssell, Kurt
 CORPORATE SOURCE: Univ. Stockholm
 SOURCE: Acta Chem. Scand. (1962), 16, 87-93
 DOCUMENT TYPE: Journal
 LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB cf. CA 49, 10214c. The asym. borospiroans (I) and (II) were prepared as MePrPh(PhCH₂)N⁺ salts. 1-(2-Bromophenyl)-2-bromonaphthalene (III) is prepared by diazotizing 8.5 g. 1-(2-aminophenyl)-2-naphthylamine. A Hg complex of the diazonium salt is formed by adding Hg NO₃)₂ and KBr (Schwechten, CA 27, 69) yielding on decomposition and distillation 4 g. III, b₂ 203-4°. 1-(2-Iodophenyl)-2-iodonaphthalene (2 g.) (Cava and Stucker, CA 50, 8579a) dissolved in 15 mL. Et₂O is treated with 9 mL. N BuLi at -30 to -40° and then with 0.43 g. BF₃.Et₂O in 5 mL. Et₂O. After evaporating Et₂O and adding EtOH (30 mL.), 0.8 g. methylpropylbenzylphenylammonium α-bromo-d-camphor-π-sulfonate (IV) (Wedekind and Froehlich, Ber. 38, 3438 (1905)) is added causing a precipitation of 0.1 g. I, m. 203-4° (MeNO₂), [α]_D -91°. II is prepared from 2-[4,2-Me(Br-Mg)C₆H₃O]C₆H₄MgBr (Campbell, CA 41, 3469f) and BF₃.Et₂O in THF.

Addition of IV in EtOH solution causes precipitation of II, m. 187-91° (MeNO₂-EtOH), [α]_D -42°. MePrPh(PhCH₂)NI (V), [α]_D -69°, is prepared by reaction of IV with LiI in Me₂CO, m. about 160° (decomposition). mMeC₆H₄(p-ClC₆H₄)BOPr (VI), b.p. 172-4°, is obtained in 71% yield by treating m-MeC₆H₄B(OPr)₂ with p-ClC₆H₄MgBr in Et₂O at -60°. After hydrolyzing with chilled dilute H₂SO₄ VI is extracted with Et₂O and distilled

IT 205-10-7, 7H-Benzo[b]naphtho[1,2-d]borole
(spiro derivative)
RN 205-10-7 HCAPLUS
CN 7H-Benzo[b]naphtho[1,2-d]borole (8CI, 9CI) (CA INDEX NAME)



CC 33 (Organometallic and Organometalloidal Compounds)

IT 205-10-7, 7H-Benzo[b]naphtho[1,2-d]borole
(spiro derivative)

L12 ANSWER 76 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1962:66979 HCAPLUS

DOCUMENT NUMBER: 56:66979

ORIGINAL REFERENCE NO.: 56:12918d-e

TITLE: Aminoditolylborane and the preparation of diarylborinic acids

AUTHOR(S): Coates, G. E.; Livingstone, J. G.

CORPORATE SOURCE: Durham Coll., UK

SOURCE: Journal of the Chemical Society (1961) 4909-11
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

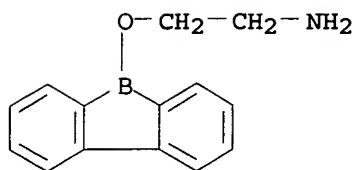
LANGUAGE: Unavailable

AB The following route to diarylborinic acids was investigated: BCl₃ + Ph₂NH → Cl₂BNPh₂ (I). I + ArMgX → Ar₂BNPh₂ (II). II + H₂O + H₂NCH₂CH₂OH → Ar₂BOCH₂CH₂NH₂ (III). III + HCl → Ar₂BOH. Only a slight excess of Grignard reagent is used, making this procedure more economical than present ones. The yields of III are in the range of 51-93% and there is no contamination by boronic acids. The following new acids and their 2-aminoethyl esters were prepared (R in R₂BOR'); o-MeOC₆H₄, m.p. of ester 164-5°; PhC.tplbond.C, m.p. of ester 172-4°, of acid 98-100°; 3,4-Me₂C₆H₃, m.p. of ester 204-6°.

IT 97176-42-6, Ethylamine, 2-[(5H-dibenzoborol-5-yl)oxy]-
(preparation of)

RN 97176-42-6 HCAPLUS

CN Ethylamine, 2-[(5H-dibenzoborol-5-yl)oxy]- (7CI) (CA INDEX NAME)



CC 33 (Organometallic and Organometalloidal Compounds)
 IT 524-95-8, Borinic acid, diphenyl-, 2-aminoethyl ester 2622-89-1,
 Borinic acid, diphenyl- 6962-82-9, Borinic acid,
 bis(p-bromophenyl)-, 2-aminoethyl ester 6962-88-5, Borinic acid,
 di-1-naphthyl-, 2-aminoethyl ester 13025-77-9, Borane,
 aminodi-o-tolyl- 19565-45-8, Borinic acid, di-p-tolyl-,
 2-aminoethyl ester 61733-90-2, Borinic acid,
 bis(p-chlorophenyl)-, 2-aminoethyl ester 62981-91-3, Borinic
 acid, di-1-naphthyl- 66117-64-4, Borinic acid, di-p-tolyl-
 73774-44-4, Borinic acid, di-o-tolyl- 75018-24-5, Borane,
 aminodimesityl- 89566-59-6, Borinic acid, bis(p-chlorophenyl)-
 96484-29-6, Borinic acid, bis(p-bromophenyl)- 97176-42-6
 , Ethylamine, 2-[(5H-dibenzoborol-5-yl)oxy]- 97176-42-6,
 5H-Dibenzoborole, 5-2-aminoethoxy)- 97339-50-9, Borinic acid,
 bis(phenylethynyl)- 97881-32-8, Borinic acid, di-o-tolyl-,
 2-aminoethyl ester 97979-12-9, Borinic acid,
 bis(o-methoxyphenyl)-, 2-aminoethyl ester 98693-26-6, Borinic
 acid, bis(phenylethynyl)-, 2-aminoethyl ester 99269-70-2,
 Borinic acid, di-3,4-xylyl-, 2-aminoethyl ester 102032-41-7,
 Borinic acid, bis(4-biphenyl)-, 2-aminoethyl ester
 (preparation of)

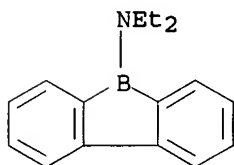
L12 ANSWER 77 OF 77 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1960:44693 HCAPLUS
 DOCUMENT NUMBER: 54:44693
 ORIGINAL REFERENCE NO.: 54:8842f-i,8843a-c
 TITLE: Synthesis and structure of aromatic boron
 compounds
 AUTHOR(S): Davidson, J. M.; French, C. M.
 CORPORATE SOURCE: Queen Mary Coll., London
 SOURCE: Journal of the Chemical Society (1960) 191-5
 CODEN: JCSOA9; ISSN: 0368-1769
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB 10-Hydroxy-9-oxa-10-boraanthracene (I) was prepared and its aromatic
 character demonstrated by ultraviolet spectroscopy. The mechanism
 of the reaction of Bu metaborate (II) with Grignard and Li
 reagents was investigated and the conditions under which organic
 boronous or boronic acid was the predominant product were examined
 An attempt to prepare 9-diethylamino-9-borafluorene was also
 described. PhMgBr (from 15.7 g. PhBr) in 50 ml. Et₂O treated
 dropwise under reflux with 10 g. phenylboronic anhydride (III) in
 75 ml. C₆H₆, refluxed a further 0.5 hr., the mixture hydrolyzed with
 200 ml. 15% HCl, the solvents removed, 20 ml. ligroine added, and
 the mixture filtered gave 3.5 g. III, m. 214°. Removal of
 the solvent from the filtrate gave 11.5 g. diphenylboronous acid
 (IV), n_D²⁰ 1.5907. IV with HOCH₂CH₂NH₂ formed 65% 2-aminoethyl
 diphenylboronite, m. 187°. 2-Biphenylphenylboronous acid
 (V) was similarly prepared from 7.5 g. III and 1 mole
 2-biphenylmagnesium iodide in Et₂O, after hydrolysis,
 ethanolamine added, and crystallized to give 10.2 g.

2-aminoethyl-2-biphenyl phenylboronite (VI), m. 175° (alc.). VI (3 g.) shaken with 30 ml. Et₂O and 30 ml. 10% HCl gave 2.55 g. V, viscous liquid. Mg (0.7 g.) reacted readily with 7.5 g. 2-iododiphenyl ether and 3 g. II in 60 ml. Et₂O after addition of iodine; after 10 min. of spontaneous refluxing and 0.5 hr. of heating the mixture was hydrolyzed with 100 ml. 15% HCl, the acid products extracted with 5% NaOH, and the basic extract acidified to give 1.5 g. o-phenoxyphenylboronic acid, m. 114° (C₆H₆-cyclohexane). 9-Bromophenanthrene (5 g.) and 2.5 g. II gave 2.45 g. 9-phenanthrylboronic acid, m. 324° (H₂O). 2,2'-Dilithiodiphenyl ether in 156 ml. Et₂O treated during 10 min. with 6.7 g. II in 25 ml. Et₂O, the solution refluxed 2 hrs., and hydrolyzed with 100 ml. 10% HCl gave 5.9 g. 10-hydroxy-9-oxa-10-boraanthracene (VII), m. 285° (C₆H₆-cyclohexane). The same solution of 2,2'-dilithiodiphenyl ether (600 ml.) and 200 ml. ether solution containing 37 g. BF₃-Et₂O simultaneously added to 100 ml. Et₂O under N during 45 min. and the mixture refluxed 1 hr. gave 11.1 g. VII. 2-Biphenylmagnesium iodide (from 10 g. 2-iodobiphenyl) in 50 ml. Et₂O treated rapidly with 3.5 g. II in 15 ml. Et₂O, and the solution refluxed 0.5 hr. gave 5 g. 2-biphenylboronic acid (VIII), m. 121-3° (H₂O), resolidified to the anhydride, m. 195°. VIII (3.9 g.) esterified with alc. by azeotropic distillation gave 3.4 g. di-Et ester, b₄ 136-8°, n₂₀D 1.5444. Di-Bu 2-biphenylboronate (IX) was prepared by direct esterification of the Grignard reaction mixture after hydrolysis. 2-Iodobiphenyl (26.5 g.) and 8.8 g. II afforded 13.3 g. IX, b_{0.6} 149-51°, n₂₀D 1.5310. IX (7.5 g.) heated 18 hrs. at 140° with 11 g. PCl₅ gave 4.35 g. 2-biphenylboron dichloride, b_{0.25} 95-6°, n₂₀D 1.5661. 2,2'-Dilithiobiphenyl (from 4 g. 2,2'-diiodobiphenyl) in 60 ml. Et₂O slowly treated with 0.9 g. II in 15 ml. Et₂O under N, the solution refluxed 15 min., hydrolyzed with dilute NH₄Cl, and the solution azeotropically distilled with HOCH₂CH₂NH₂ and PhMe gave 1.3 g. bis(2-aminoethyl)2-biphenyl boronate, m. 134° (C₆H₆). A sample was hydrolyzed with dilute HCl to the acid which was dried to form the anhydride, m. 206° (cyclohexane).

IT 97322-63-9, 5H-Dibenzoborole, 5-diethylamino-
(attempted preparation of)
RN 97322-63-9 HCAPLUS
CN 5H-Dibenzoborol-5-amine, N,N-diethyl- (9CI) (CA INDEX NAME)



CC 10G (Organic Chemistry: Heterocyclic Compounds)
IT 97322-63-9, 5H-Dibenzoborole, 5-diethylamino-
(attempted preparation of)